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COMPARISON OF THE NATIONAL URANIUM TAILINGS PROGRAM'S PROBABILISTIC CODE UTAP2 WITH ATOMIC ENERGY OF CANADA LIMITED'S PROBABILISTIC CODE SYVAC3-UT2

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ABSTRACT

This report describes a comparison of the output of two codes: UTAP2 (Uranium Tailings Assessment Program, Version 2) and SYVAC3 (Systems Variability Analysis Code, generation 3). Both codes are probabilistic systems assessment codes, written to serve as tools in the preparation of long-term environmental assessments. Both codes consist of a central core of 'executive' modules, to which are linked one or more submodels that are representative of the physical system being assessed.

UTAP2 has been developed for use in environmental assessments of the impact of uranium tailings.[1] Available documentation for this assessment includes a description of the model representing the tailings site. From these written descriptions, a set of model-related specifications were created, that provide a detailed description of the uranium tailings model.

The specifications were used to develop the system model code for use with SYVAC3. The resultant code, SYVAC3-UT2, was then compared with UTAP2 for three different simulations.

This report describes the steps used to prepare the specifications and prepare the tailings model code for SYVAC3-UT2. Results are also described from the comparisons of UTAP2 and SYVAC3-UT2.

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EXECUTIVE SUMMARY

This report describes a comparison of two probabilistic assessment codes applied to an assessment of a hypothetical uranium tailings system. The two codes are the Uranium Tailings Assessment Program, Version 2 (UTAP2) and the third generation of the Systems Variability Analysis Code, (SYVAC3).

UTAP2 was developed by SENES Consultants, under contract to the National Uranium Tailings Program. SENES also applied a version of the code in a preliminary study of a uranium tailings system (SENES, 1986). SYVAC3 was developed by Atomic Energy of Canada Limited, as a long-term assessment tool for the study of nuclear fuel waste disposal. Previous generations of SYVAC3 have been applied to several interim studies of waste disposal concepts, including a comparison with a prior version of UTAP (Goodwin and Andres, 1986).

This code intercomparison exercise was undertaken to contribute to the quality assurance of UTAP2. The first task in this contract was to develop a complete set of specifications for the uranium tailings model, based on the documentation prepared by SENES (1986). The specifications were then used to develop SYVAC3-UT2, which consists of the SYVAC3 executive modules combined with the uranium tailings model. This independent coding of the tailings model provides for a comprehensive test of the corresponding code in UTAP2 (as well as portions of the executive modules in UTAP2).

Comparisons were then carried out between UTAP2 and SYVAC3-UT2 using six simulations with known parameter values. Each of the first three simulations involved cycles of detailed comparison, investigation of differences and modification of the specifications and SYVAC3-UT2. The last three simulations were only used to compare results. The agreement between the results given by the two codes improved substantially between the first and final comparisons. The results of the final comparisons showed that the first and last four of the simulations were in "excellent" agreement, while the second was in "good" agreement, according to the comparison criteria established for this code intercomparison.

Over the course of the project, 177 ambiguities, questions, and problem areas were documented. Approximately one hundred were resolved in setting up the specifications for the uranium tailings model. The remainder were detected and rationalized during the comparison of UTAP2 and SYVAC3-UT2. All such questions are noted in this report, along with the steps undertaken to address them.

The project took more time and money than originally estimated, primarily for three reasons. First, the model proved to be much more complicated than we estimated from a review of the preliminary documentation. The specifications eventually contained over 250 diagrams, compared to an anticipated 100. Second, there were delays in receiving final documentation from which to construct specifications. In some cases, the preliminary documentation changed substantially, and affected completed specifications and code. Third, there were more discrepancies between the UTAP2 code and documentation than we expected. We found and corrected differences at a rate of from one to three per day, and so the comparison

phase took several weeks. Some parts of the original scope of the project were not completed (notably the comparison of a set of probabilistic simulations), even with increases to the budget and adjustments to the schedule.

The following general conclusions are made:

(1) We have identified the majority of the significant differences between the documentation and the code for the uranium tailings model in UTAP2, as evidenced by the agreement between the UTAP2 and SYVAC3-UT2 results. This process contributes to the quality assurance of UTAP2 since the differences can be readily resolved through appropriate corrections to the code and/or documentation. Once resolved, there will be increased confidence that the tailings model is correctly implemented in UTAP2. (A previous study (Goodwin and Andres, 1986) provides additional quality assurance support for the UTAP executive modules.)

(2) A comprehensive description of complex models, such as the uranium tailings model, requires the use of detailed specifications as well as the conventional written documentation. This is particularly true when it is desirable to produce a complicated code that must meet detailed quality assurance guidelines, when subsequent model and code modification are anticipated, or when such a code is to be used in a detailed code intercomparison such as the intercomparison described in this report. During the course of this project, we have prepared detailed specifications (data flow diagrams, data dependency diagrams and a data dictionary) that are an accurate description of the tailings model in SYVAC3-UT2, and that describe changes that are required to improve the consistency between the UTAP2 documentation and code.

A number of recommendations are also made that pertain to this project and to related projects undertaken in the future. The main recommendations are:

(1) All documented differences between the UTAP2 code and documentation should be re-examined and resolved by experts in the uranium tailings model. All changes should also be updated in the detailed specifications produced in this contract.

(2) Some aspects of the uranium tailings model should be examined and possibly improved upon. Of particular note are the physical and chemical discontinuities and the dependence of the results on the size of the time step.

(3) Comparisons of the type documented in this report contribute substantially to the quality assurance process, and should be repeated whenever extensive revisions are made to subsequent versions of UTAP2. Some specific recommendations are also made to make the code intercomparison process more efficient.

RÉSUMÉ

Dans le présent rapport, on décrit une comparaison de deux programmes d'évaluation probabiliste qu'on applique à l'évaluation d'un système hypothétique de résidus de traitement de l'uranium. Les deux programmes sont le Programme d'Évaluation des Résidus de traitement de l'Uranium, Version 2 (UTAP2) ainsi que la troisième génération du Programme d'Analyse de la Variabilité des Systèmes (SYVAC3).

C'est SENES Consultants qui a réalisé UTAP2 sous contrat pour le Programme National d'étude des Résidus de traitement de l'Uranium. De plus, SENES a appliqué une version du programme dans une étude préliminaire d'un système de résidus de traitement de l'uranium (SENES, 1986). C'est l'Énergie Atomique du Canada, Limitée qui a réalisé SYVAC3 comme moyen d'évaluation à long terme pour étudier l'évacuation des déchets de combustible nucléaire. On a appliqué les générations précédentes de SYVAC3 à plusieurs études provisoires de concepts d'évacuation de déchets dont une comparaison avec une version antérieure d'UTAP (Goodwin et Andres, 1986).

On a entrepris cet exercice d'intercomparaison de programmes pour contribuer à l'assurance de la qualité d'UTAP2. Le premier travail contractuel a été d'établir une série complète de prescriptions pour le modèle de résidus de traitement de l'uranium d'après la documentation rédigée par SENES (1986). On s'est ensuite servi des prescriptions pour réaliser SYVAC3-UT2 composé des modules directeurs de SYVAC3 conjugués au modèle des résidus de traitement de l'uranium. Ces programmes indépendants du modèle de résidus assurent un essai complet du programme correspondant dans UTAP2 (ainsi que des parties des modules directeurs dans UTAP2).

On a ensuite fait des intercomparaisons d'UTAP2 et SYVAC3-UT2 à l'aide de six simulations à valeurs paramétriques connues. Chacune des trois premières simulations a comporté des cycles de comparaison minutieuse, l'étude des différences et la modification des prescriptions et de SYVAC3-UT2. Les trois dernières simulations n'ont servi qu'à comparer les résultats. L'accord entre les résultats des deux programmes s'est beaucoup amélioré entre les première et dernière comparaisons. Les résultats des dernières comparaisons ont montré que la première et les quatre dernières de la série de simulations ont été en "excellent" accord tandis que la deuxième a été en "bon" accord suivant les critères de comparaison établis pour l'intercomparaison des codes.

Au cours du projet, on a documenté 177 ambiguités, questions et points difficiles. On en a résolu à peu près cent lors de l'établissement des prescriptions pour le modèle de résidus de traitement de l'uranium. On a décelé ou rationalisé le reste lors de la comparaison d'UTAP2 et de SYVAC3-UT2. On a noté toutes les questions de ce genre dans le présent rapport ainsi que les mesures prises pour les aborder.

Ce projet a demandé plus de temps et coûté plus cher qu'on ne l'avait d'abord prévu, principalement pour les trois raisons suivantes: premièrement, le modèle s'est avéré être beaucoup plus compliqué que nous ne l'avions prévu d'après un examen de la documentation préliminaire; les prescription ont comporté en fin de compte plus de 250 schémas alors qu'on en avait prévu 100, deuxièmement, il y a eu des retards dans la réception

de la documention finale d'après laquelle on a établi les prescriptions; dans certains cas, la documentation préliminaire a changé considérablement et influencé les prescriptions et le programme achevés; troisièmement, il y a eu plus de différences entre le programme UTAP2 et la documentation que nous ne l'avions prévu. Nous avons trouvé et corrigé des différences à raison d'une à trois par jour - la phase de comparaison a donc demandé plusieurs semaines. Certaines parties du plan original n'ont pas été achevées (notamment la comparaison d'une série de simulations probabilistes) même en augmentant le budget et en modifiant le calendrier des travaux.

On a tiré les conclusions générales suivantes:

(1) nous avons identifié dans UTAP2 la plupart des grandes différences entre la documentation et le programme pour le modèle des résidus de traitement de l'uranium comme le prouve l'accord entre les résultats d'UTAP2 et de SYVAC3-UT2. Ceci contribue à l'assurance de la qualité d'UTAP2 du fait qu'on peut facilement résoudre les différences en apportant des corrections appropriées au programme et/ou à la documentation. Lorsqu'elles seront résolues, on sera plus certain que l'application du modèle de résidus dans UTAP2 est correcte. (Une étude précédente (Goodwin et Andres, 1986) apporte un appui supplémentaire de l'assurance de la qualité pour les modules directeurs d'UTAP);

(2) une description complète des modèles complexes tels que le modèle des résidus de traitement de l'uranium, demande l'emploi de prescriptions précises ainsi que de la documentation écrite classique. Ceci est surtout vrai lorsqu'il est souhaitable de produire un programme compliqué devant suivre des règles directrices précises d'assurance de la qualité, lorsqu'on prévoit un modèle et une modification de programme ultérieurs ou quand on doit employer ce programme dans une intercomparaison précise de codes telle que celle décrite ici. Au cours du projet, nous avons rédigé des prescriptions précises (schémas de cheminement des données, schémas de dépendance des données et dictionnaire des données) qui décrivent exactement le modèle des résidus de SYVAC3-UT2 ainsi que les modifications qu'il faut apporter à la documentation d'UTAP2 et/ou au programme pour que le programme soit en accord la documentation d'UTAP2.

En outre, on a fait un certain nombre de recommandations se rapportant à ce projet et à des projets connexes à entreprendre dans l'avenir. Les recommandations principales sont suivantes:

(1) toutes les différences documentées entre le programme UTAP2 et la documentation devraient être ré-examinées et résolues par des experts en modèle de résidus de traitement de l'uranium. De plus, toutes les modifications devraient être mise à jour dans les prescriptions précises produites dans le cadre du contrat;

(2) certains points du modèle de résidus de traitement de l'uranium devraient être examinés et éventuellement améliorés. À noter en particulier les discontinuités physiques et chimiques et la dépendance des résultats par rapport à l'étendue de l'échelon de temps;

(3) les comparaisons du type qui est documenté dans ce rapport contribuent beaucoup au processus de l'assurance de la qualité et devraient être répetées toutes les fois qu'on apporte des révisions poussées aux versions suivantes d'UTAP2. De plus, on fait certaines recommandations particulières pour rendre plus efficace le processus d'intercomparaison des programmes.

1.0 INTRODUCTION

1.1 Background

The National Uranium Tailings Program (NUTP) was set up to sponsor research and development directed at Canada's uranium mill tailings. One of NUTP's main goals is to investigate and develop procedures for the long-term environmental assessment of the disposal of uranium mill tailings (Harrison et al., 1985). The probabilistic systems assessment approach was chosen for development, since this approach can address the uncertainty and variability inherent in a disposal system that will operate far into the future.

The probabilistic assessment approach relies heavily on numerical simulations to produce system performance predictions. Mathematical models are developed for all processes that could significantly influence the behaviour of the disposal system and its potential impacts on man. Uncertainty and variability of the parameters in the mathematical models are accounted for by describing them in terms of suitable probability density functions, representing the range and probabilities of feasible values for the parameters over the period of interest.

The mathematical complexity of the models and data requires the use of advanced numerical algorithms implemented on a digital computer. An important aspect of such work is the verification of these models and the associated computer codes. Verification describes the processes undertaken at each stage in the development of the computer code to prevent the introduction of error. For example, verification steps ensure that specifications match the conceptual model, and that code matches specifications. This report also uses the term "code quality assurance" to denote the collection of verification steps used to ensure that the final computer code accurately represents the specified models and data.

Verification of a probabilistic assessment model can be achieved by several possible techniques. This report describes the technique in which two independently-developed codes are applied to the same problem, using identical models, followed by a detailed comparison of their results. This approach is of particular value for codes that are very complicated from a logical and/or numerical point of view. The uranium tailings model requires such a complicated code, and the main objective of this report is to describe such a comparison. Another objective is to describe the quality assurance procedures to show that the code developed, as part of this contract, is an accurate representation of the uranium tailings model.

The two codes being compared are the Uranium Tailings Assessment Program, Version 2 (UTAP2) and the SYstems Variability Analysis Code, generation 3 (modified to include the uranium tailings model). Both codes are probabilistic systems assessment codes, consisting of a set of executive models linked with a set of system-specific submodels. UTAP2 was developed for the NUTP by SENES (1986), following a previous version (UTAP; see SENES (1985)) for application to assessments of uranium mill tailings. SYVAC3 was developed by Atomic Energy of Canada Limited (AECL) as an assessment tool for the long-term assessment of the disposal of nuclear fuel waste (SYVAC3 was preceded by two earlier versions: SYVAC1 (Dormuth and Sherman, 1981) and SYVAC2 (Sherman et al., 1986)).

The executive modules in SYVAC3 consist of about 10 000 lines of code which have been developed using an extensive set of quality assurance procedures. The executive modules in SYVAC3 were developed so that the code could be readily adapted to assessments other than nuclear fuel waste disposal. In this report, SYVAC3 is linked with the tailings model originally developed for UTAP2 (SENES, 1986), and the combination of executive modules and tailings models is known as SYVAC3-UT2.

1.2 Scope of Work

The main objective of this study was to compare simulation results from UTAP2 with simulation results from SYVAC3-UT2. This comparison provides an independent check of UTAP2 and contributes to its quality assurance.

In addition, however, it became apparent that a second major objective was the preparation of a complete set of specifications (data flow diagrams, data dependency diagrams and a data dictionary) for the uranium tailings model. In our previous comparison, for example, we recommended that written documentation of the tailings model should be supplemented with detailed specifications, such as data flow diagrams and a data dictionary (Goodwin and Andres, 1986). The increased complexity of the tailings model in UTAP2 has led us to believe that detailed specifications are essential. These specifications play an important role in the quality assurance of the model and code, since they bridge the gap between the scientific description and the working code. These specifications would also be a very useful element for subsequent modification to the model and/or code by other research groups.

To achieve these two main objectives, the project was broken into five main tasks. They were defined as follows:

(1) Produce a complete set of specifications for the uranium tailings model, using the available documentation for Phase III and ancillary information from SENES Consultants, as required. The specifications should be kept up to date throughout the project. For example, all changes and additions that occur to the original specifications should be reflected in the final specifications, including documentation describing what has been changed, and the reasons for the change.

(2) From the specifications, prepare FORTRAN code of the model and implement it in SYVAC3-UT2. Also prepare an APL equivalent version of the model for testing and comparison. Compare the APL and FORTRAN versions using a randomly-selected simulation. Continue with code modification and comparison until the two versions produce equivalent results, and are consistent with the specifications from task (1). The development of FORTRAN code should follow documented software standards and quality assurance procedures as described below. The comparison of the FORTRAN code and the APL code is used to ensure that the uranium tailings model included in SYVAC3-UT2 meets the reference specifications. This task was performed in the previous UTAP - SYVAC3 comparison (Goodwin and Andres, 1986), and proved to be a very powerful quality assurance procedure.

(3) Compare the results from SYVAC-UT2 with the results from UTAP2 for six deterministic simulations (a deterministic simulation is one in which the parameter values are known, and not sampled randomly from the parameter probability distributions). Resolve all discrepancies until the two codes agree to within specified comparison criteria for major output variables. Specification of comparison criteria and the selection of variables to be compared should be made in consultation with SENES consultants and the Scientific Authority. The six deterministic runs are to be used to resolve all major discrepancies between the tailings model used in UTAP2 and SYVAC3-UT2, and could require the detailed comparison of intermediate variables, as well as the "final" variables such as pH and total dose. Comparisons of the six deterministic runs is to proceed in a sequential fashion; that is all discrepancies are to be resolved for the first deterministic run before the second run is begun. At the end of task (3), results for all six deterministic runs are to agree to within the specified comparison criteria.

(4) Repeat the comparison of results from SYVAC3-UT2 with the results from UTAP2 for a probabilistic case containing at least 500 simulations. Resolve all discrepancies until the statistics of the two codes agree to within specified comparison criteria for major output variables. Specification of comparison criteria and the selection of variables to be compared should be made in consultation with SENES consultants and the Scientific Authority. The probabilistic case involves a comparison of statistical results from UTAP2 and SYVAC3-UT2 and provides for quality assurance of the uranium tailings model over a wide range of sampled parameters. In addition, the comparison of the probabilistic results provides for an overall quality assurance of UTAP2 since all components of the code are involved (including some executive modules that perform functions such as parameter sampling).

(5) Prepare a report documenting the code development and the results of the comparison, and present a seminar on the project to NUTP personnel in Ottawa. The report is to contain descriptions of the APL-FORTRAN comparison and the deterministic and probabilistic comparisons of UTAP2 and SYVAC3-UT2. Full documentation of the specifications should be provided, including a record of any modifications that were made during the course of the contract work.

Task (1) required extensive input from SENES consultants. A series of letters and telephone conversations took place, in which questions and answers were exchanged relating to the uranium tailings model. Appendix A contains a record of all ancillary explanations required to produce the complete set of specifications.

Task (1) also proved to be much more difficult than was originally expected. As a consequence, budgeting and scheduling constraints had a significant effect on the degree of completion of the remaining tasks. In task (2), it became necessary to drop those elements involving APL. In task (3), we were able to complete the six deterministic simulations, but were unable to resolve all major discrepancies. We were also unable to perform the probabilistic comparison in task (4). Finally, in task (5), we were unable to schedule a seminar on the project.

Despite these shortcomings, we feel that several important goals were achieved. As discussed below, these goals include the preparation of a complete set of specifications for the uranium tailings model and the identification and documentation of a large number of flaws in UTAP2 and/or in the documentation of UTAP2. The majority of such flaws have been identified, as shown by the good agreement reached between UTAP2 and SYVAC3-UT2 results. Resolution of these flaws will increase the confidence that the uranium tailings model has been correctly implemented in UTAP2.

1.3 Quality Assurance Procedures

Much of the time spent on this study was used to develop detailed specifications of the uranium tailings model. During this development, it was important to ensure that the specifications were an accurate representation of the documented tailings model, and that the code developed for SYVAC3-UT2 was a faithful representation of the specifications. To meet these requirements, a set of quality assurance procedures was applied. These procedures included the following:

(1) A formal and comprehensive set of specifications were prepared to define the code required for use with SYVAC3. The requirements for the code were taken from the SENES report (SENES, 1986), together with ancillary information provided by SENES (see Appendix A). The specifications for the uranium tailings model used with SYVAC3 are reproduced in Appendix B, which includes data flow and data dependency diagrams. Appendix C contains a copy of the data dictionary, which is an integral component of the specifications.

(2) Walkthroughs were held for all specifications produced. Members at the walkthroughs included experts not directly involved with this project. To expedite the walkthrough process, some of the later walkthroughs involved only two or three participants. In each case, however, a formal record was taken of all participants and of all relevant comments made. A final sign-off was required for the final walkthroughs of all figures, confirming that all major problems had been resolved.

(3) The late arrival of some ancillary information had unexpected consequences; for example, a response to one question changed previously-accepted specifications for several component models. To ensure that all such changes were correctly made, a final repeat walkthrough of all specifications was held.

(4) The specification, design and coding phases of the project were assigned to different individuals. The designer and programmer worked from the specifications only, and provided additional "design walkthroughs" and "code walkthroughs". All problems encountered were relayed back to the analyst, so that the specifications could be revised as required. Most problems encountered at the design and code phases were detailed and very specific.

(5) PC-OUTLINE (BBS, 1986) was used as a design tool. This software product proved to be very useful in the production of structured and modular design. In turn, an orderly and logically-organized design promotes quality assurance of the subsequent code.

(6) Three separate compilers were used for FORTRAN code. A VAX mainframe compiler was used on draft code as it was written. The IBM Professional FORTRAN compiler (PROFORT, 1984) was used in early development after the code had been moved to a COMPAQ microcomputer. The Lahey F77L compiler (Lahey, 1986) was used for later development on the COMPAQ because of its source language debugger. The use of distinct compilers provides additional confidence that the code has been correctly implemented. The use of several compilers also lends confidence in the portability of the code between different computers.

(7) During the previous comparison of UTAP and SYVAC3 (Goodwin and Andres, 1986), it was noted that the initial conditions for some differential equations were not defined. The uranium tailings model in UTAP2 contains a large number of coupled differential and/or difference equations, and in some cases it was not clear whether all required initial conditions had been provided. The code was therefore designed to preset all time-dependent variables to "negative infinity" (i.e. -1.0 E37). Subsequent calculations would then quickly expose any missing initial conditions, since unusual results would be calculated using this value.

(8) All FORTRAN code was developed following ANSI FORTRAN 77 standards, and other coding standards established for the Canadian Nuclear Fuel Waste Management Program (Hoffman and Sherman, 1985). In addition, SYVAC3 has predefined procedures for the linkage of submodels to the executive modules, and for the format of input files (see, for example, Goodwin and Andres, 1986). Development of these linkages and input files was facilitated through the use of code and file "templates".

2.0 DEVELOPMENT OF THE TAILINGS MODEL CODE FOR SYVAC3-UT2

2.1 Overview of the Tailings Model

The uranium tailings model used here was developed by SENES Consultants, and has been documented in detail (SENES, 1986). Some of the overall features of the model are as follows:

(1) The radionuclides considered are natural uranium, total thorium, radium-226, radon-222 and lead-210.

(2) Water pathways include a user-specified river-lake system downstream from the tailings site. The rivers and lakes are linked together through a set of node points.

(3) Atmospheric pathways are modelled using a sector-ring coordinate system. There are 16 sectors corresponding to wind roses, and up to 5 rings. The distance between the rings is user-specified, with a minimum inner ring radius of 1 km and a maximum outer ring radius of 50 km.

(4) Dose calculations can be carried out for both a critical receptor and an average receptor.

(5) Dose calculations consider dose due to ingestion, inhalation and external exposure. Doses due to ingestion include ingestion of contaminated drinking water, fish, above- and below-ground vegetables and meat from caribou and moose. Doses due to inhalation include inhalation of radon gas and its daughters, and inhalation of contaminated dust. Dose due to external exposure deals with groundshine from dust deposited on soil.

(6) The pH of lakes downstream from the tailings pile is calculated taking into consideration dissolved concentrations of calcium, iron, sulphate and aluminum.

Figure 1 shows a simplified conceptual structure of the uranium tailings model (see Appendix B for a detailed description of data flow diagrams). It consists of 14 major component modules, where module is defined here to mean one or more related processes required to produce one or more major calculated variables. The lowest level module, TSOURC, produces calculated variables required by higher levels of modules which in turn may produce variables required by the next level of modules, and so forth. The uppermost level modules, DOSE and LAKEPH, produce the final major variables of interest, which include the total annual average effective whole body dose equivalent commitment[1] to a receptor, and the pH of the lakes downstream from the tailings site.

Figure 1 is a substantial simplification of the actual model for the uranium mill tailings system. A more complete set of figures for the system is given in Appendix B.

Most of the documentation for these modules is found in the SENES report (SENES, 1986). Some additional information is reproduced in Appendix A of this report. A brief description of the function of each of these modules is given below.

TSOURC: This is the tailings 'source term' module, which provides the waterborne and airborne source term variables that are required by the GWATER, WATEX, EROS, RADON and DUST modules. It represents the evolution in time of the tailings site, and includes an unsaturated zone and a saturated zone. Processes that are modelled include (SENES, 1986):

(1) Oxidation of pyrite within the unsaturated zone. It is assumed that all pyrite within the unsaturated zone is exposed to oxygen which diffuses into the tailings from the atmosphere. As the pyrite is oxidized, it produces sulphate ions, which migrate downward towards the saturated zone.

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[1] referred to as dose in the rest of this document

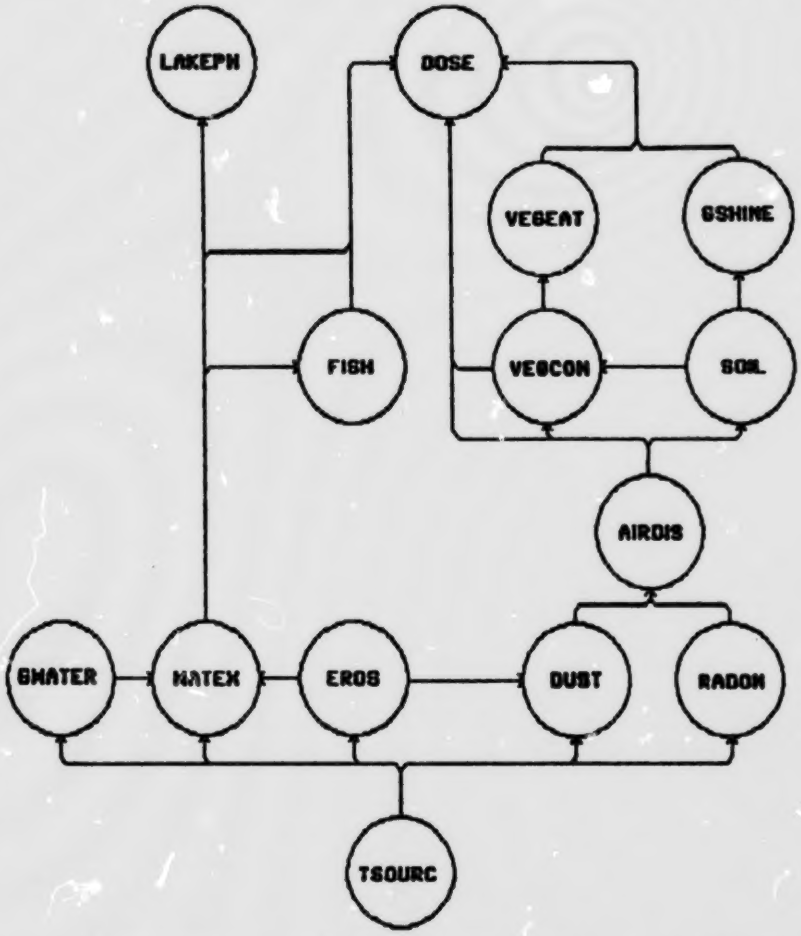


Figure 1. Simplified Data Flow Diagram of the Uranium Tailings Model. Circles represent clusters of related processes. Arrows represent major variables being passed from one process to another.

(2) Dissolution of gypsum within the upper layer of the unsaturated zone. The constant influx of fresh water from rainfall and melting snow gradually dissolves the gypsum in the unsaturated zone. At the start of the simulation, it is assumed that the entire unsaturated zone contains a uniform distribution of gypsum. As time progresses, the gypsum in the upper layer dissolves and moves towards the saturated zone. The upper layer is also referred to as the gypsum-depleted layer, the sulphate-depleted layer and layer 1.

(3) Precipitation of gypsum within the lower layer of the unsaturated zone. Dissolved gypsum from the upper layer of the unsaturated zone moves down into the lower layer of the unsaturated zone, along with sulphate ions from the oxidation of pyrite. The presence of these 'excess' sulphate ions causes some gypsum (a hydrated calcium sulphate) to reprecipitate. The lower layer is also referred to as the gypsum-enriched layer, the sulphate-enriched layer and layer 2.

(4) Movement of the front between the upper and lower layers of the unsaturated zone. At the start of the simulation, there is no 'upper' layer. As the gypsum at the top of the unsaturated zone dissolves and moves downwards, the upper (gypsum-depleted) layer is gradually formed. The remaining lower portion of the unsaturated zone, the lower (gypsum-enriched) layer, is gradually reduced with time. After some time, the front reaches the interface between the unsaturated and saturated zone. At this time, only the upper (gypsum-depleted) layer remains.

(5) Modifications to the rate of dissolution, movement and precipitation of gypsum due to the addition of limestone. The most obvious effect of the addition of limestone is to raise the pH from the acidic range (due to the oxidation of pyrite) towards a neutral range. The rate of oxidation of pyrite is also reduced, and the equilibrium between gypsum and its component ions is shifted (less sulphate is released).

(6) Changes in concentration of ions in the saturated zone. The upper part of the saturated zone, also referred to as layer 3 and the mixing layer, receives contaminants from the lower layer of the unsaturated zone. Water moves from layer 3 horizontally to surface waters and vertically to groundwaters. The saturated zone below layer 3 is referred to as layer 4, and is effectively equivalent to a deep groundwater layer.

(7) Changes to the pH of the four layers that make up the tailings pile. Calculations of pH take into consideration changing concentrations of calcium and sulphate ions, and various equilibria between gypsum, gibbsite, kaolinite, iron (III) hydroxides, and carbonic acid/dissolved carbon dioxide. Modifications are also provided to account for the addition of limestone to the tailings.

(8) Changing concentrations of dissolved uranium in the four layers. The source of the dissolved uranium is essentially assumed to be the two unsaturated layers, where uraninite dissolves in conjunction with the oxidation of pyrite. Uranium concentrations in the saturated layers is controlled by downward movement of water containing dissolved uranium, including a factor accounting for sorption.

(9) Changing concentrations of thorium in the four layers. The concentration of thorium is assumed to be controlled by the solubility of $Th(OH)_4(s)$, taking into consideration pH and sulphate concentrations (with an upper limit of 5×10^{-5} mol dm^{-3}). Sorption in the saturated layers is not modelled.

(10) Changing concentrations of radium-226 in the four layers. One source of radium-226 is ingrowth from the decay of thorium-230. The second major source of radium-226 is assumed to be its presence as a solid solution end member in barite (crystalline barium sulphate). Barite is assumed to behave like gypsum, with a barite-depleted layer and a barite-enriched layer in the unsaturated zone. There is also a barite front, lagging behind the gypsum front, that moves downwards to the saturated zone. Radium is assumed to dissolve and precipitate in association with barite in the unsaturated zone (layers 1 and 2). In the saturated zone (layers 3 and 4) the calculations for radium-226

include ingrowth from thorium-230, dissolved radium moving downwards from other layers, sorption of radium, and decay of radium-226 to radon-222.

(11) Changing concentrations of lead-210 in the four layers. It is assumed that lead-210 and other lead isotopes are ideally mixed, with concentrations of lead in solution controlled by the solubility of lead sulphate. Calculations in the unsaturated zone include lead sulphate-depleted and -enriched layers, and a moving front. Lead-210 concentrations are given by the solubility of lead sulphate scaled by the relative abundance of lead-210, and augmented by the ingrowth of lead-210 from the decay of radium-226. Calculations in the saturated zone include ingrowth from radium-226, dissolved lead-210 moving downwards from other layers, sorption of lead, and decay of lead-210.

TSOURC requires about 47 different input parameters, including the time step-size (DT) and the net precipitation (NPRCP) (see the entries for PCHEMS, PPBS, PRAS, PTHS and PUS in the Data Dictionary, Appendix C). It produces a large number of output variables, including:

(1) Time-dependent solid phase concentrations of uranium, thorium, lead-210 and radium-226 in the uppermost layer of the unsaturated zone (layer 1), for use in the DUST, RADON and EROS modules.

(2) Time-dependent solid phase concentrations of radium-226 in the lower layer of the unsaturated zone (layer 2), for use in the RADON module.

(3) Time-dependent aqueous phase concentrations of uranium, thorium, lead-210, radium-226, calcium and sulphate in the mixing layer of the saturated zone (layer 3), for use in the WATEX module.

(4) Time-dependent aqueous phase concentrations of uranium, thorium, lead-210 and radium-226 in the bottom layer of the saturated zone (layer 4), for use by the GWATER module.

TSOURC produces a number of other output variables, as shown in the detailed specifications. TSOURC is described in figures 0.0 and 1.0 through to 1.5.3.8 of the specifications (see Appendix B). Figures 1.6 through to 1.6.3.10 also contain elements of the tailings source term (and are described below in the EROS module).

GWATER: This module describes the subsurface transport of contaminants from the bottom of the saturated zone (layer 4) and subsequently discharging into the watershed. The module includes:

(1) Estimates for the average seepage of contaminants out of the tailings pile and entering a groundwater flow system.

(2) A mass balance equation for contaminant flow. A homogeneous, isotropic semi-infinite medium is modelled with terms for dispersion, advection, sorption and decay. (Radionuclide chains are not modelled.)

(3) Modifications to approximate a time-varying source term. The variable inlet boundary condition is modelled using discrete time-steps, the

principle of superposition and a Green's function solution to the mass balance equation.

(4) An approximation for the ingrowth of Pb-210 from the decay of Ra-226.

GWATER requires 16 input parameters, including 4 nuclide-dependent decay constants, 4 nuclide-dependent distribution coefficients and the time step-size (DT) (see the entry for PGWAT in the Data Dictionary, Appendix C). Its major output is

(1) Time-dependent concentrations of uranium, thorium, radium-226 and lead-210 at the discharge point of the aquifer into the watershed, for use in WATEX.

GWATER is described in figures 3.0 and 3.1 to 3.1.7 of the specifications (see Appendix B).

WATEX: This module describes the transport of contaminants through a watershed downstream from the tailings pile. The watershed is modelled as a series of user-specified rivers and lakes. Each river and lake is defined by an end node, with a total of 10 nodes available (the first node must be a river). Features of this module include:

(1) A simple hydrologic model of water flows past each node.

(2) Changes in concentration of calcium and sulphate ions in the river and lakes due to inflow by surface and subsurface waters, and dilution by other waters in the watershed.

(3) Changes in concentration of uranium, thorium, radium-226 and lead-210 in the watershed. A simple dilution model is used for the rivers. A more complex model is used for the lakes, that takes into consideration sorption of radionuclides onto lake sediments. The lake model also has terms to describe desorption of a fraction of the sorbed radionuclides (the remaining fraction is assumed to be irreversibly sorbed), and to approximate radioactive decay chains.

(4) Contamination of the watershed through surface water flows, groundwater seepage and erosion. The first node in the watershed is assumed to receive contaminated surface water flowing out of the tailings site. It is also assumed that the first river/lake in the watershed can receive additional contaminants from groundwater flow and from erosion.

(5) Contamination of aquatic vegetation (macrophytes). A simple equilibrium model is used, which requires the average concentrations, over the entire watershed, of uranium, thorium, radium-226 and lead-210. Aquatic vegetation is assumed to be a foodstuff for moose living in the watershed.

WATEX requires 38 input parameters, including 24 used to define an 8-node watershed and the time step-size (DT) (see entry for PWATEX in the Data Dictionary, Appendix C). The major output variables produced by WATEX are:

(1) Time-dependent aqueous concentrations, at each watershed node, of uranium, thorium, radium-226 and lead-210, for use in the DOSE module.

(2) Time-dependent aqueous concentrations, at each watershed node, of calcium and sulphate ions, for use in the LAKEPH module.

(3) Time-dependent concentrations (watershed averages) of uranium, thorium, radium-226 and lead-210 in aquatic vegetation and in water for use in the VEGEAT module.

WATEX is described in figures 3.0 and 3.3 to 3.3.9 in the specifications (see Appendix B).

EROS: This module describes the erosion of the tailings pile, followed by the transport of tailings solids to the first downstream node in the watershed. The EROS module could also be considered as part of the TSOURC module, since it provides a source term for surface water transport. It has been separated out in Figure 1, however, since the processes it represents are significantly different from the rest in TSOURC. The features of EROS include:

(1) Modelling of erosion using a modified version of the Universal Soil Loss Equation (USLE). The USLE is an empirical equation for predicting soil loss from water erosion, with parameters that include slope of the tailings pile, a soil erodibility factor and a "control practice" parameter.

(2) The effect of tailings vegetation. The fraction of the tailings pile that is vegetated affects the selection of the "control practice" factor, and is calculated as a function of the pH of the surface layer of the tailings.

EROS requires 14 input parameters including the time step-size (DT) (see the entry for PEROS in the Data Dictionary, Appendix C). Its major output is:

(1) Total time-dependent sediment mass leaving the tailings pile due to erosion, for use in WATEX.

EROS is described in figures 1.0 and 1.6 to 1.6.3.10 in the specifications (see Appendix B).

LAKEPH: This module describes the affects of the tailings pile on the pH of the lakes in the watershed. In principle, it could be considered as part of the WATEX module, but it has been separated out in Figure 1 since lake pH is one of the major output variables from the tailings model. The LAKEPH module calculates the time-dependent changes in the pH of the watershed, taking into account calcium and sulphate concentrations, and thermodynamic equilibria for aluminum and iron species. It requires 30 input parameters, including 24 parameters used to define an 8-node watershed, the time step-size (DT) and the net precipitation (NPRCP) (see the entry for PLAKPH in the Data Dictionary, Appendix C). The major output variables are

(1) Time-dependent pH of each of the lakes in the watershed.

The pH of the lakes are major output variables of the tailings model. Lake pHs are also used elsewhere in the tailings model (not shown in Figure 1), such as in calculating fish availability (in the DOSE modules).

LAKEPH is described in figures 3.0 and 3.2 to 3.2.7 of the specifications (see Appendix B).

FISH: This module provides a description of the effect of the tailings on fish populations living in the downstream watershed. Features of this module include:

(1) Estimates of the effect of pH on the availability of game fish, at all nodes in the watershed.

(2) Bioaccumulation of uranium, thorium, radium-226 and lead-210 in fish flesh, for fish located at all nodes in the watershed.

The FISH MODEL requires 4 input parameters. It produces two major output variables, which are:

(1) Time-dependent concentrations of uranium, thorium, radium-226 and lead-210 in fish located at each node in the watershed, for use in the DOSE module.

(2) Time-dependent fractions of fish available at each node in the watershed, relative to the normal population of fish, for use in the DOSE module.

FISH is described in figures 4.1.5 and 4.1.5.1 to 4.1.5.2 of the specifications (see Appendix B).

RADON: This module describes the release of gaseous Rn-222 from the tailings pile to the air immediately above. It is assumed that radon is released only from the unsaturated zone. Processes that are modelled in RADON include:

(1) Emission of Rn-222 from the upper (gypsum-depleted) layer of the unsaturated zone. The flux of Rn-222 is a function of the depth of the upper layer and the concentration of Ra-226 within the upper layer.

(2) Emission of Rn-222 from the lower (gypsum-enriched) layer of the unsaturated zone. This flux of Rn-222 is a function of the depths of the lower and upper layers, and the concentration of Ra-226 within the lower layer.

(3) The effect of moisture content on the radon diffusion coefficient. Increased moisture in the tailings reduces radon diffusion; radon gas does not diffuse through water.

The RADON module requires 8 input parameters (see the entry for PRADON in the Data Dictionary, Appendix C). It produces one variable which is:

(1) The annual average emission rate of Rn-222 gas from the tailings unsaturated zone (upper and lower layers) as a function of time, for use in the AIRDIS module.

RADON is described in figures 2.0 and 2.2 to 2.2.4 in the specifications (see Appendix B).

DUST: This module describes the saltation of the tailings pile, and calculates the release of uranium, thorium, radium-226 and lead-210 contained within dust particles to the air immediately above the tailings pile. Processes that are modelled in DUST include:

(1) Release of dust particles to the air. This is due to wind erosion, and is a function of parameters such as the particle size and mean wind speed.

(2) Changes to the rate of emission of contaminants to the air above the tailings pile. Emission rates are assumed to be equal to the emission rates of dust particles released from the tailings pile multiplied by the concentrations of uranium, thorium, radium-226 and lead-210 in the upper layer of the unsaturated zone.

(3) changes to the amount of exposed tailings surface area as a function of time. This parameter is provided by the EROS module.

The DUST module requires 5 input parameters (see the entry for PDUST in the Data Dictionary, Appendix C). It produces one variable which is:

(1) Time-dependent emission rates of uranium, thorium, radium-226 and lead-210 in dust from the tailings surface, for use in AIRDIS.

DUST is described in figures 2.0 and 2.1 in the specifications (see Appendix B).

AIRDIS: This module describes the atmospheric transport of radon gas and contaminants in dust particles from the tailings pile. Radon gas and contaminated dust can be inhaled by a receptor and contaminated dust can fall on vegetation and soil. The processes modelled in AIRDIS include the following:

(1) Dispersion of contaminants in air by diffusion and advection. A Gaussian plume model is used, with 16 sectors and 5 rings for a total of 80 sites for which air concentrations are calculated. The model also calculates average concentrations for the watershed area and the study area.

(2) Corrections for a distributed source. This correction provides for the treatment of the tailings as an area source instead of a point source.

(3) Changes in the concentrations of radon-222, uranium, thorium, radium-226 and lead-210 in air at a receptor. These concentrations are calculated using the Gaussian plume model and the emission rates of radon

gas and the uranium, thorium, lead-210 and radium-226 in dust at the tailings pile.

AIRDIS requires 9 input parameters, including the STAR wind data (see the entry for PAIRDS in the Data Dictionary, Appendix C). The major calculated output variables from AIRDIS are:

(1) Time-dependent average annual concentrations of uranium, thorium, radium-226 and lead-210 associated with dust in air at 80 sites around the tailings source, for use in the VEGCON, SOIL and DOSE modules.

(2) Time-dependent average annual concentration of radon-222 gas in air at 80 sites around the tailings source, for use in DOSE modules.

(3) Time-dependent average annual concentrations of uranium, thorium, radium-226, and lead-210 in dust, and of radon-222 in air for the entire watershed area and for the entire study area, for use in the DOSE and VEGCON modules.

AIRDIS is described in figures 2.0 and 2.3 to 2.3.7 in the specifications (see Appendix B).

VEGCON: This module calculates the concentration of contaminants in five types of locally-grown vegetation. Contaminated vegetation can then affect man through direct ingestion, or through ingestion of moose and/or caribou which have fed on the vegetation. Features of the VEGCON module include:

(1) Contamination by airborne dust particles. Dust from the tailings pile containing uranium, thorium, radium-226 and lead-210 can contaminate the vegetation by direct foliar retention, or by root uptake from contaminated soils. VEGCON uses air concentrations and soil concentrations (in the root zone) that are calculated in the AIRDIS and SOIL modules.

(2) Changes in concentration of uranium, thorium, radium-226 and lead-210 in the edible portions of the vegetation. This process takes into account parameters such as yield density and the duration of exposure of the vegetation.

(3) Modelling of 5 different classes of vegetation. These classes include:
    - Above-ground and below-ground vegetables that are directly consumed by man. Air and soil concentrations are required at each of the 80 receptor sites modelled by AIRDIS.
    - Summer forage crops (grasses) which are ingested by migratory caribou. The air and soil concentrations required for this class of vegetation are the averages of the entire study area.
    - Browse vegetation, which are meant to include only terrestrial vegetation ingested by moose (the WATEX module models aquatic vegetation). The air and soil concentrations required for this class of vegetation are the averages for the watershed area.
    - Lichens which are ingested by migratory caribou. This vegetation class requires only air concentrations, which are the averages for the entire study area.

VEGCON requires 48 input parameters, including 5 vegetation-specific values for 6 parameters (see the entry for PVGDEP in the Data Dictionary, Appendix C). It produces the following output variables:

(1) Time-dependent average annual concentrations of uranium, thorium, radium-226 and lead-210 in above-ground and below-ground vegetables at each of the 80 receptor sites, for use in the DOSE module.

(2) Time-dependent study-area average annual concentrations of uranium, thorium, radium-226 and lead-210 in summer forage, for use in the VEGEAT module.

(3) Time-dependent watershed-area average annual concentrations of uranium, thorium, radium-226 and lead-210 in browse vegetation and lichen, for use in the VEGEAT module.

VEGCON is described in figures 2.0 and 2.6 of the specifications (see Appendix B).

VEGEAT: This module calculates the concentrations of uranium, thorium, radium-226 and lead-210 in caribou and moose meat. It includes the following processes:

(1) Bioaccumulation of uranium, thorium, radium-226 and lead-210 in caribou meat. The sources of the contaminants are assumed to be summer forage and lichen (from the VEGCON module) and drinking water (from the WATEX module, using watershed-area averaged concentrations).

(2) Bioaccumulation of uranium, thorium, radium-226 and lead-210 in moose meat. The sources of the contaminants are assumed to be browsing vegetation (for the VEGCON module) and aquatic plants and drinking water (from the WATEX module, using watershed-area averaged concentrations).

VEGEAT uses 44 input variables that include feed-to-caribou (or -moose) meat transfer coefficients and feed ingestion rates (see the entry for PVGEAT in the Data Dictionary, Appendix C). It produces the major output variables:

(1) Time-dependent concentrations of uranium, thorium, radium-226 and lead-210 in caribou flesh, for use in the DOSE module.

(2) Time-dependent concentrations of uranium, thorium, radium-226 and lead-210 in moose flesh, for use in the DOSE module.

VEGEAT is described in figures 4.1, 4.1.2 to 4.1.2.4 and 4.1.3 to 4.1.3.2 in the specifications (see Appendix B).

SOIL: This module calculates the concentrations of contaminants in different soil layers at the 80 receptor sites. Processes included in the model are:

(1) Deposition of contaminants in dust onto the top soil layer. Uranium, thorium, radium-226 and lead-210 in airborne dust is assumed to settle onto the surface of the soil in the 80 receptor areas.

(2) Changing concentrations of contaminants in two soil layers. The calculation takes into account radioactive decay, sorption onto the solid phases, downward movement of dissolved contaminants to subsurface layers, and contaminant removal from the soil due to leaching by surface runoff waters.

SOIL uses 26 input parameters including the time step-size (DT) (see the entry for PSOIL in the Data Dictionary, Appendix C). It produces the following output variables:

(1) Time-dependent concentrations of uranium, thorium, radium-226 and lead-210 in the first subsurface soil layer (layer 2, also known as the root zone) of all 80 receptor sites, for use in the GSHINE and VEGCON modules.

(2) Time-dependent concentration of uranium, thorium, radium-226 and lead-210 in the top soil layer of all 80 receptor sites, for use in the GSHINE module.

SOIL is described in figures 2.0 and 2.4 to 2.4.6 in the specifications (see Appendix B).

GSHINE: This module calculates the external dose rate due to groundshine. GSHINE could be considered as part of the dose module, but it has been separated in Figure 1 since it uses substantially different mathematical equations. The calculations include consideration of:

(1) Concentrations of uranium-238,, thorium, radium-226, lead-210 and radon-222 in the soil layers. The uranium-235 decay chain is not considered.

(2) An approximation for shielding by overlaying soil layers and gamma-ray flux loss due to emanation and removal of radon gas.

(3) Different energy bands in the decay chains. Up to 5 energy bands for each of 5 radionuclide chains are considered.

GSHINE uses 10 input parameters (see PGSHIN in the Data Dictionary, Appendix C). It includes 25 energy bands (see ENERGY(nuc,band) in the Data Dictionary) and 25 "total gamma rays" (see NDEC(nuc,band) in the Data Dictionary). The output from this module is one of the major outputs from the uranium tailings model, and is:

(1) Time-dependent total groundshine dose rate at all 80 receptor locations, summed over all decay chains.

GSHINE is described in figures 2.0 and 2.5 to 2.5.7 in the specifications (see Appendix B).

DOSE: This is the dose module, describing the radiological impact to a receptor due to the presence of a nearby uranium tailings pile. Processes modelled in DOSE include (SENES, 1985):

(1) Radiological impact due to the ingestion of uranium, thorium, radium-226 and lead-210 in contaminated vegetation, caribou meat, moose meat, fish and drinking water from a lake.

(2) Radiological impact due to the inhalation of dust containing uranium, thorium, radium-226 and lead-210 and the inhalation of radon-222 and its daughters.

(3) Consideration of the relevant characteristics of a "critical" and an "average" receptor. These characteristics include diet and location within the study area.

DOSE requires approximately 40 input parameters (see the entries for PING and PINH in the Data Dictionary, Appendix C). Some of these parameters depend on factors such as whether the receptor is a critical or an average receptor. DOSE also requires the 4 "location" parameters (LOCF, LOCV, LOCW and LOCA) which define where the receptor is exposed to contaminated fish, vegetables, water and air. It produces a number of variables that are major output variables from the uranium tailings model:

(1) Time-dependent average annual dose due to the ingestion of uranium, thorium, radium-226 and lead-210 in above-ground and below-ground vegetables.

(2) Time-dependent average annual dose due to the ingestion of uranium, thorium, radium-226 and lead-210 in caribou and moose meat.

(3) Time-dependent average annual dose due to the ingestion of uranium, thorium, radium-226 and lead-210 in drinking water from a lake.

(4) Time-dependent average annual dose due to the ingestion of uranium, thorium, radium-226 and lead-210 in fish flesh.

(5) Time-dependent average annual dose due to the inhalation of uranium, thorium, radium-226 and lead-210 in dust.

(6) Time-dependent average annual dose due to the inhalation of radon gas and its radioactive daughters.

(7) Time-dependent average annual dose due to groundshine exposure from uranium-238, thorium, radium-226 and lead-210.

(8) Time-dependent total annual internal dose due to the ingestion, inhalation and groundshine exposure of uranium, thorium, radium-226 and lead-210 and inhalation of radon-222.

DOSE is described in figures 0.0 and 4.0 to 4.4 in the specifications (see Appendix B).

2.2 Overview of SYVAC3

The SYstems Variability Analysis Code (SYVAC) has been developed as an assessment tool for use within Canada's Nuclear Fuel Waste Management Program. SYVAC provides a methodology, based on systems variability analysis (Dormuth and Quick, 1981), for treating variability and uncertainty in long-term assessments of different waste disposal concepts (Goodwin et al., 1987).

Figure 2 provides an illustration of the SYVAC concept with submodels that are appropriate for the assessment of the Canadian concept for nuclear fuel waste disposal (other submodels are used for other disposal concepts). Information from the research program, detailed analysis and expert opinion are used to develop simplified models and data that represent the system. As shown in Figure 2, the disposal system has been divided into submodels for the vault, geosphere and biosphere. Uncertainty and variability in the data are accommodated by the use of probability distributions to define parameter values, rather than a single "best estimate" or "worst case" value. SYVAC selects a simulation defined to be a possible state of the system, by randomly sampling a value for each parameter from its specified distribution. This set of parameter values is then used within the submodels to estimate the transport of contaminants from the vault to the biosphere, and leads to a predicted impact for that simulation. The selection and prediction process is repeated, typically a thousand times or more, and the results are summarized in, for example, a histogram of predicted consequence versus their frequency of occurrence.

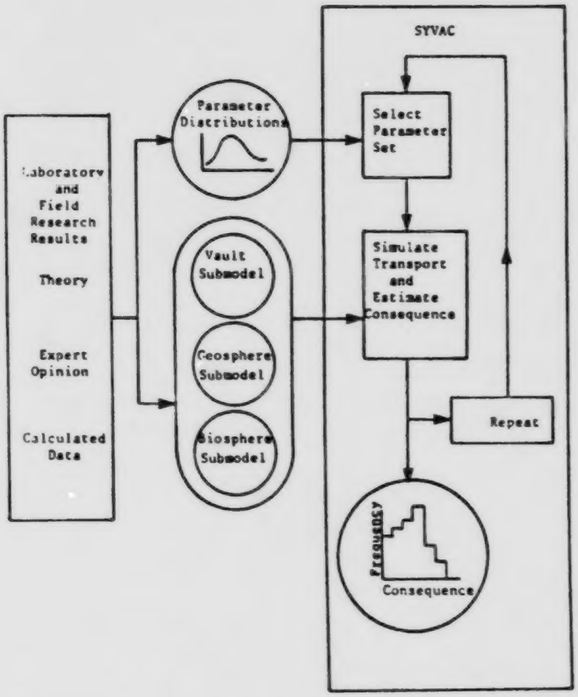

SYVAC
Laboratory and Field Research Results
Theory
Expert Opinion
Calculated Data
Parameter Distributions
Vault Submodel
Geosphere Submodel
Biosphere Submodel
Select Parameter Set
Simulate Transport and Estimate Consequence
Repeat
Frequency
Consequence

Figure 2: Schematic Overview of the SYVAC Assessment Approach

In this manner, SYVAC produces a distribution of estimates of impact that reflects a measure of the uncertainties associated with the predicted impacts.

The development of SYVAC has proceeded in a step-wise fashion. The first generation of SYVAC, SYVAC1 (Dormuth and Sherman, 1981), has been applied to several preliminary assessments (Wuschke et al., 1981; Wuschke et al., 1983; Guvanasen, 1985). The second generation, SYVAC2 (Sherman et al., 1986), has also been used in several assessment studies (Wuschke et al., 1985; Goodwin et al., 1987).

Work is now underway for the development of SYVAC3. For this generation of the code, considerable effort is being devoted to the development of improved submodels for the Canadian nuclear fuel waste management program. It was recognized, however, that changes were also required to the SYVAC executive modules, principally to expedite the substitution of new submodels into the overall code (Goodwin, 1984). This requirement is represented in figure 2, which shows that the SYVAC executive modules are conceptually independent of the system models and the associated data.

A considerable amount of effort is now being devoted to the quality assurance of the SYVAC3 executive module (Goodwin et al., 1987). Although all modules have not yet passed the complete set of quality assurance procedures, a tested and working version of SYVAC3 has been available for some time.

The flexibility of SYVAC3 has been demonstrated by unpublished work for the Canadian Nuclear Fuel Waste Management Program, in a contract report for the NUTP (Murray et al., 1986), and in a previous comparison study performed for the NUTP (Goodwin and Andres, 1986). To distinguish between these different applications, the acronym for SYVAC3 has been slightly modified. SYVAC3-CC3, for example, is the version of SYVAC3 containing the third version of submodels required to assess the Canadian concept for nuclear fuel waste disposal. For the studies described in this report, the full designation is SYVAC3-UT2, where UT2 denotes the application to the second version of NUTP's model for uranium tailings (and as contained in UTAP2).

2.3 Specifications

An essential component of the quality assurance of a computer code is the specification of the requirements of the code. Specifications are used to demonstrate that a systems analysis has been carried out, and that the requirements desired can be achieved. Ideally, the complete set of specifications can be handed over to a designer and programmer, who should be able to produce the desired code without referring to any other related material. Development of suitable specifications is a time-consuming process, but there are positive returns, since the time spent on specifications means less time is required for the programming stage, and since a better quality product is produced.

We have also concluded that a complete set of specifications are essential for projects such as this one, where a computer code must be developed for a complicated mathematical model. In general, the available documentation (SENES, 1986) of the uranium tailings model provides a comprehensive scientific description of the model. However this documentation is inadequate for the purpose of developing a computer code. Appendix A, for example, lists over 170 comments that refer to deficiencies in the documentation, including documentation that is ambiguous, missing and incorrect. Most of these deficiencies were noted during the preparation of the specifications, because this task imposed a logical and thorough approach to the model definition.

The detailed specifications produced in this contract also had a number of other benefits, including:

(1) The uranium tailings model contains many calculated variables that are frequently entwined in a complex fashion. The data flow diagrams provide a concise description of how these variables interact, and greatly facilitated the code design phase.
(2) Many of the variables are calculated from solutions or approximations to differential equations. The data dependency diagrams were particularly useful in detecting those equations for which the initial conditions were missing.
(3) During the testing phase, differences between UTAP2 and SYVAC3-UT2 could frequently be due to one or more parts of a long chain of computations. The specifications (and the code design) provided a powerful logical basis from which the source of these differences could be identified.

We feel that it would not have been possible to develop and test SYVAC3-UT2 without these specifications, unless there existed an established team of modelling and programming experts.

For this project, it only remained to develop suitable specifications for the uranium tailings model. The uranium tailings model was largely documented in Volume 3 of the SENES report (SENES, 1986), and this material served as the starting point for the preparation of specifications. During the first attempts at producing specifications, and also at subsequent stages, it was found that some additional information was required. Most of the required information was provided by B.E. Halbert and others from SENES Consultants, and is reproduced in Appendix A.

Several interim versions of these specifications were prepared before the final product was produced. The interim versions were subjected to formal walkthroughs to ensure that the specifications developed accurately reflect the uranium tailings model. These walkthroughs were successful in detecting many errors in the specifications before they had a deleterious impact on the programming stage. The walkthroughs were also useful in producing a self-contained and consistent set of specifications that were suitably customized to match the requirements of the project. A summary of the walkthroughs of the specifications is reproduced in Appendix D.

These interim specifications were not yet final. During the testing and comparison phases of this project, many differences were detected in the results of UTAP2 and SYVAC3-UT2 that affected the specifications (see Appendix A, item 21, comments 105 and upwards). We established the policy that changes to SYVAC3-UT2 would be performed only from its specifications. As a consequence the interim specifications were always kept up-to-date with SYVAC3-UT2.

The final set of specifications for the uranium tailings model are presented in Appendices B and C. Appendix B contains the set of data flow diagrams, and data dependency diagrams. Appendix C contains the data dictionary, another important product of the quality assurance process.

Finally, we note that the specifications produced successfully met their objectives. Both the designer and programmer were able to perform their tasks without referencing any of the original SENES documentation. Furthermore neither the designer nor the programmer were experts in any of the component models that were coded.

2.4 Design of the Tailings Model for Use in SYVAC3-UT2

The design phase of SYVAC3-UT2 development produced working documents from which the code was developed.* Unlike the model specifications, this documentation was not required in the formal documentation, but rather was a scaffolding to assist in the assembly of the code. These documents were kept up-to-date only until a working version of the code was completed.

There were two major objectives of the design phase. The first objective was to develop a structure for the tailings model code. The second objective was to design data structures for the storage of model data in the code.

Design of Code Structure

The design of the structure for the tailings model code used in SYVAC3-UT2 had to meet three constraints. These constraints were:

(1) The code should implement the tailings model as defined by the specifications.

(2) The code should have a standard interface with the SYVAC3-UT2 executive (for more explanation, see, for example, Goodwin and Andres, 1986).

(3) The code should be divided into sections with minimal data coupling between them, so that differences between UTAP2 and SYVAC3-UT2 could be localized to the part of the code where the differences originated.

The design of the tailings model code for SYVAC3-UT2 proceeded in three stages: review of data flow diagrams, creation of an initial structure, and refinement of the structure.

In the first stage of code design, data flow diagrams of the tailings model were condensed onto two pages, one for calculations that were not time related (Figure 3), and one for time-dependent calculations (Figure 4).

---

* Not all of the uranium tailings model was coded and tested. The portion of the model dealing with dose due to external groundshine was omitted because the specifications for this part of the model were finalized very late in the project.

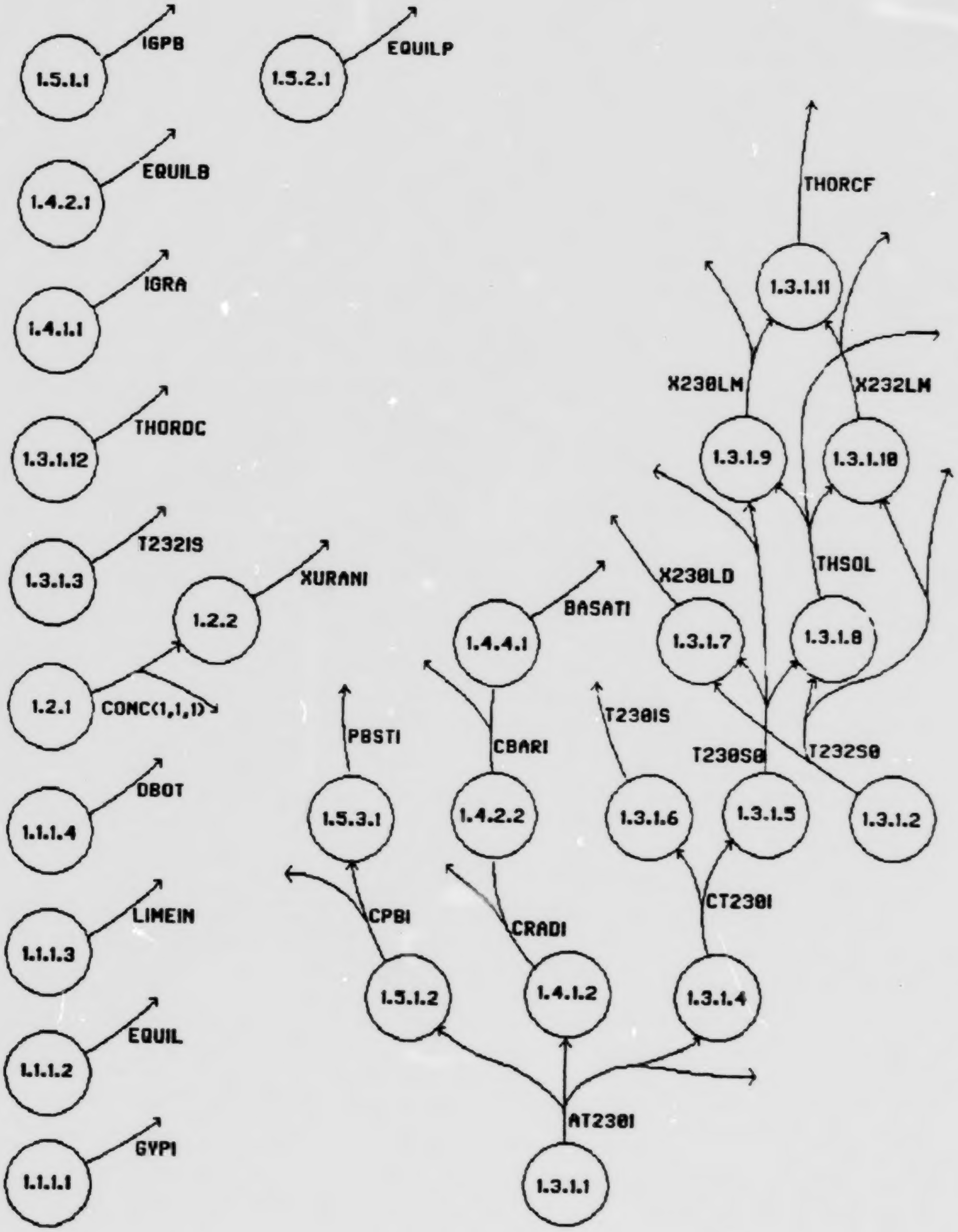

1.5.1.1
IGPB
1.5.2.1
EQUILP
1.4.2.1
EQUILB
1.4.1.1
IGRA
1.3.1.12
THORDC
1.3.1.3
T232IS
1.2.1
CONC(1,1,1)
1.2.2
XURANI
1.1.1.4
DBOT
1.1.1.3
LIMEIN
1.1.1.2
EQUIL
1.1.1.1
GYPI
THORCF
1.3.1.11
X230LM
X232LM
1.3.1.9
1.3.1.10
THSOL
X230LD
1.3.1.7
1.3.1.8
BASATI
1.4.4.1
PBSTI
CBARI
T230IS
T230S0
T232S0
1.5.3.1
1.4.2.2
1.3.1.6
1.3.1.5
1.3.1.2
CPBI
CRADI
CT230I
1.5.1.2
1.4.1.2
1.3.1.4
AT230I
1.3.1.1

Figure 3: Detailed Data Flow Diagrams for Time-Independent Calculations

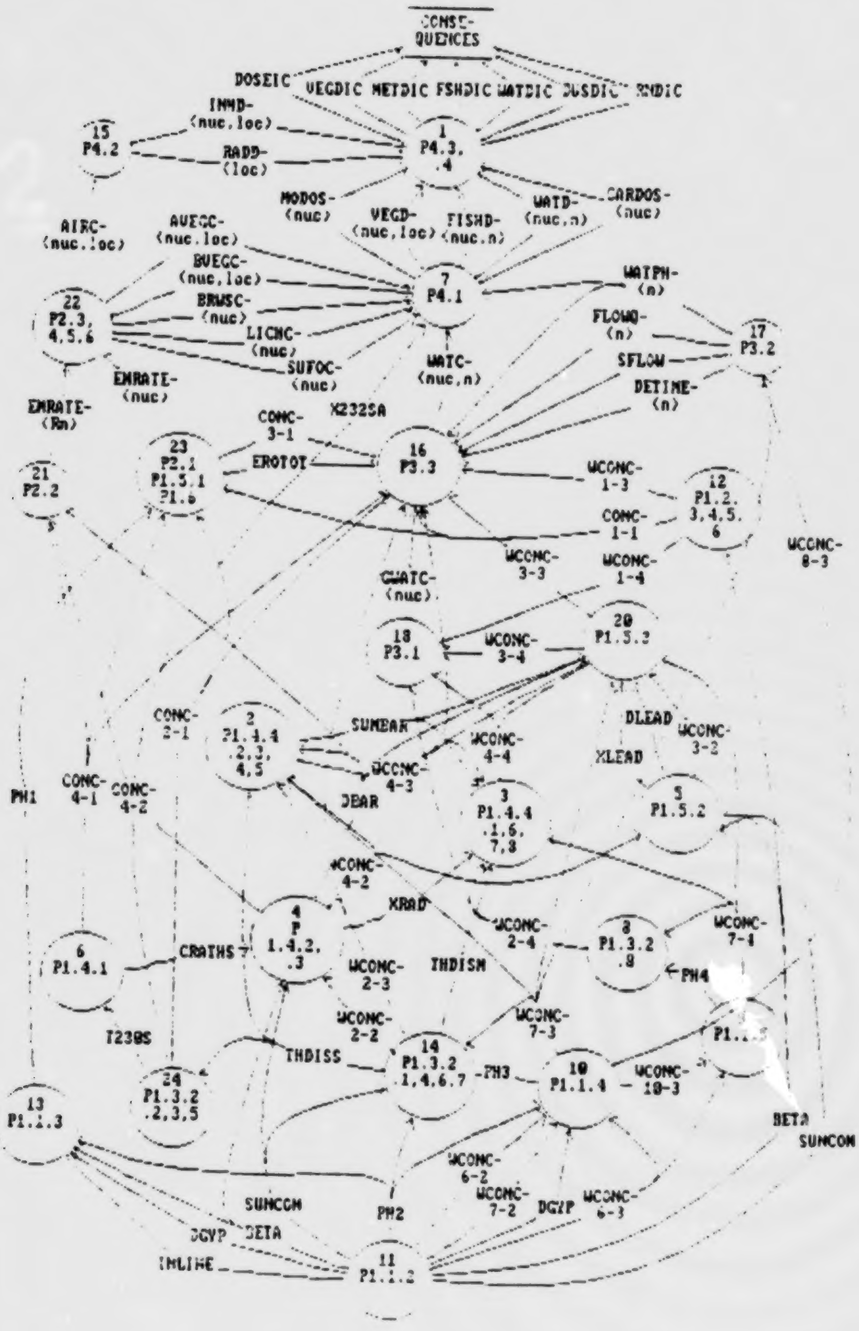

CONSE-
QUENCES
DOSEIC
VEGDIC
METDIC
FSHDIC
WATDIC
DUSDIC
RNDIC
15
P4.2
INHD-
(nuc,loc)
RADD-
(loc)
1
P4.3,
.4
MODOS-
(nuc)
VEGD-
(nuc,loc)
FISHD-
(nuc,n)
WATD-
(nuc,n)
CARDOS-
(nuc)
AIRC-
(nuc,loc)
AVEGC-
(nuc,loc)
BVEGC-
(nuc,loc)
BRWSC-
(nuc)
LICNC-
(nuc)
SUFOC-
(nuc)
22
P2.3,
4,5,6
7
P4.1
WATPH-
(n)
FLOWQ-
(n)
SFLOW
DETIME-
(n)
17
P3.2
WATC-
(nuc,n)
EMRATE-
(nuc)
EMRATE-
(Rn)
CONC-
3-1
X232SA
EROTOT
16
P3.3
21
P2.2
23
P2.1
P1.5.1
P1.6
WCONC-
1-3
CONC-
1-1
12
P1.2.
3,4,5.
6
WCONC-
8-3
WCONC-
3-3
WCONC-
1-4
GWATC-
(nuc)
18
P3.1
WCONC-
3-4
20
P1.5.3
CONC-
2-1
2
P1.4.4
.2,3,
4,5
SUMBAR
WCONC-
4-4
WCONC-
4-3
DLEAD
WCONC-
3-2
XLEAD
PH1
CONC-
4-1
CONC-
4-2
DBAR
3
P1.4.4
.1,6,
7,8
5
P1.5.2
WCONC-
4-2
XRAD
4
P
1.4.2,
.3
WCONC-
2-4
8
P1.3.2
.8
WCONC-
7-4
6
P1.4.1
CRATHS
WCONC-
2-3
THDISM
PH4
WCONC-
2-2
WCONC-
7-3
T238S
THDISS
14
P1.3.2
.1,4,6,7
PH3
10
P1.1.4
WCONC-
10-3
13
P1.1.3
24
P1.3.2
.2,3,5
BETA
SUNCON
WCONC-
6-2
WCONC-
7-2
DGYP
WCONC-
6-3
SUNCON
PH2
DGYP
BETA
INLIME
11
P1.1.2

Figure 4: Detailed Data Flow Diagrams for Time-Dependent Calculations

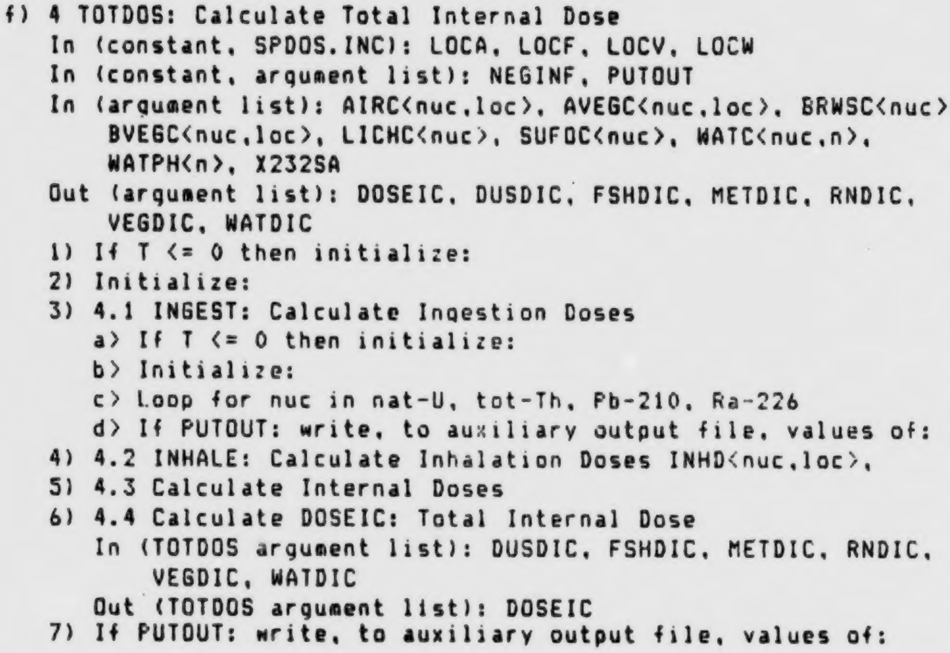
The aim in creating these diagrams was to show enough detail to define an appropriate code structure, without showing so much detail that the overall data flow through the model would be lost. The chief source of difficulty in this stage was the high degree of coupling (i.e., the large number of data flows) among parts of the model. Some variables were even defined recursively. For example, the variable PH2 was expressed in terms of the variable INLIME, which in turn was expressed as a function of PH2. While such feedback loops are realistic in that feedback occurs in natural processes, they are difficult to work with in a computer model.

In the second stage of code design, an initial structure was developed by mapping the data flow diagram onto a set of subroutines. Usually such a mapping takes advantage of natural clusters in the data flow diagram to divide the processing. In this case, the model was so highly connected that little clustering was observed. It was therefore decided to use a simple functional breakdown. There were four main subroutines: SOUCON to calculate source concentrations, ATMCON to calculate atmospheric concentrations, WATERS to perform river and lake calculations, and TOTDOS to calculate dose estimates. There were also a number of lower level subroutines that were called by these four.

One particular decision that was taken at this point was to use a sequence of fixed time steps in the simulation (as in UTAP2). SYVAC3 has a comprehensive set of time series routines that use variable-length time steps as required to represent functions with a prescribed accuracy. However, the SYVAC3 time series routines were not appropriate for this application because many parts of the uranium tailings model are explicitly dependent on DT, the time-step size.

In the final stage of code design, the code structure was refined and filled out in detail using an outliner called PC-OUTLINE (BBS, 1986). An outliner is a software package that displays text on a computer screen in point form. Each point has subpoints and text which may or may not be displayed. There can be several levels of subpoints arranged in a hierarchy. An outliner generally has powerful commands for reorganizing the structure of the point hierarchy, and so it is a good tool for reviewing and organizing information. In this case, a hierarchical code outline was constructed, showing for each subroutine and for each major block of code within a subroutine, the inputs, outputs, and common blocks needed. Each block was cross-referenced back to the specifications. It was possible to try many different structures for the code before settling on a final design, by taking advantage of the outliner's ability to rearrange a hierarchy.

Figure 5 shows a small part of the code design for the uranium tailings model, namely the highest level design for the subroutine TOTDOS. Lower level structure has been shown for point 3) only, but the other points have such structure as well. Most points have only one line of text shown. The major point f) and point 6) are exceptions. The text associated with these points has been printed to show the inputs and outputs.



```
f) 4 TOTDOS: Calculate Total Internal Dose
   In (constant, SPDOS.INC): LOCA, LOCF, LOCV, LOCW
   In (constant, argument list): NEGINF, PUTOUT
   In (argument list): AIRC<nuc,loc>, AVEGC<nuc,loc>, BRWSC<nuc>,
       BVEGC<nuc,loc>, LICHC<nuc>, SUFDC<nuc>, WATC<nuc,n>,
       WATPH<n>, X232SA
   Out (argument list): DOSEIC, DUSDIC, FSHDIC, METDIC, RNDIC,
       VEGDIC, WATDIC
   1) If T <= 0 then initialize:
   2) Initialize:
   3) 4.1 INGEST: Calculate Ingestion Doses
      a> If T <= 0 then initialize:
      b> Initialize:
      c> Loop for nuc in nat-U, tot-Th, Pb-210, Ra-226
      d> If PUTOUT: write, to auxiliary output file, values of:
   4) 4.2 INHALE: Calculate Inhalation Doses INHD<nuc,loc>,
   5) 4.3 Calculate Internal Doses
   6) 4.4 Calculate DOSEIC: Total Internal Dose
      In (TOTDOS argument list): DUSDIC, FSHDIC, METDIC, RNDIC,
          VEGDIC, WATDIC
      Out (TOTDOS argument list): DOSEIC
   7) If PUTOUT: write, to auxiliary output file, values of:
```

Figure 5: Sample Output from an Outliner Used in the Code Design of the Uranium Tailings Model. Only a small part of the code design is shown.

Design of Data Structures

In addition to designing code structure, it was necessary to design data structures for the tailings model. Data structure design was primarily constrained by the following two factors.

(1) SYVAC3 expects parameters and consequences to be stored in named common blocks of a fixed size (Goodwin and Andres, 1986)

(2) The tailings model required knowledge of some variable values at the initial time (0 or -DT), the previous time step, and the current time step.

It was therefore decided to store time-independent variables (parameters and consequences) in named common blocks, clustered into groups that were used together, and to store time-dependent variables as vectors of length three (for initial value, previous value and current value), or as arrays with a last dimension of three. Most time-dependent variables were passed through subroutine argument lists. There were three major exceptions: pH values, concentrations of radionuclides and important ions in the aqueous phase and concentrations of radionuclides in the solid phase for the four layers in the tailings. These were stored in named common blocks.

2.5 Coding and Testing

Coding

For the most part, initial implementation of the uranium tailings model for SYVAC3-UT2 was a straightforward procedure. Twenty-five FORTRAN subroutines were coded from the design and the specifications. The design determined the overall code structure and the allocation of variables to common blocks and argument lists. The specifications stated how each variable was to be calculated. The code includes many comment statements referring back to the specifications, so that it could be easily checked.

The uranium tailings model contains an estimated 3000 to 4000 lines of executable code, and coding it took about 40 man-days. Some difficulties were encountered during the initial stages of the coding, because the entire set of specifications were not available (time constraints required that coding begin before the specifications were complete). In several instances, for example, some code had to be reworked to reflect changed specifications. In general, however, the design and specification documents performed as expected; in particular the coder, who was not a modelling expert, was able to produce the code without referencing any other material on the uranium tailings model.

Preliminary Tests

After the initial implementation of the SYVAC3-UT2 code, and before the code comparison began, a series of preliminary tests were run. It took about 15 man-days of work to test and revise SYVAC3-UT2 to the point where results could be compared with UTAP2 results. The following tests were used:

(1) SYVAC3-UT2 had to compile and run on the first (nominal value) deterministic simulation. Getting the code to compile without errors was straightforward. Making it run to a normal conclusion (i.e. without encountering run-time errors) was more difficult. One problem that was immediately obvious was due to memory shortage. The large size of the tailings model, and the decision to declare all floating point variables as double precision (whereas UTAP2 uses single precision variables), resulted in a code size that exceeded available memory (640K bytes on a COMPAQ PORTABLE 286 microcomputer). This problem was resolved primarily by reducing the size of large arrays to the minimum necessary for compatibility with UTAP2. It remained possible to support the required 222 sampled and calculated parameters, 177 constant parameters, and 150 consequences. Changing large arrays to single precision would also have solved this problem, but it was considered important to use double precision, as a check that UTAP2 results were not unduly affected by loss of precision in calculations.

(2) Special tests, using the Lahey F77L compiler (Lahey, 1986), were required to resolve a problem encountered in running SYVAC3-UT2 that was attributed to overwritten memory. Overwritten memory can occur where there are logic errors associated with arrays; for

example an attempt to save an array element such as ARRAY(101) will produce a memory overwrite if ARRAY was declared to be only 100 elements long. Such cases were encountered in SYVAC3-UT2, and caused peculiar and puzzling errors. Initial development had used the IBM Professional FORTRAN compiler (PROFORT, 1984), which does not check whether array bounds have been exceeded. To solve this problem, the code was recompiled using the Lahey F77L compiler (Lahey, 1986). This FORTRAN compiler includes automatic array bound checking that detected where such memory overwrites were occurring. It also includes a powerful source language debugger that helped resolve other problems encountered during the test phase, and significantly accelerated the rest of the development.

(3) All intermediate variables printed out had to have reasonable values. For example, many variables representing physical quantities, such as pH and contaminant concentrations, are intrinsically non-negative. Many of these variables could be checked because all time-dependent variables were assigned the starting value -10^{37}, unless the specifications provided for a specific initial value. Any computations using these artificial starting values tended to yield unusual and highly visible results. Consequently variables that had been used without prior initialization could be tracked down by this method. Many of the comments in Item 21 of Appendix A refer to the specification of initial conditions for different variables that were found to need them. These initial conditions were based on inspection of the UTAP2 code.

(4) Time independent calculations were checked by hand, and the results compared with values produced by SYVAC3-UT2. This step revealed some discrepancies in the code and in the input parameter values used.

Tests Using UTAP2 Results

After SYVAC3-UT2 passed these tests, its results were compared with UTAP2 results, which had been provided by SENES Consultants. At first it was not practical to compare UTAP2 dose outputs with SYVAC3-UT2 dose outputs. There were many discrepancies throughout the calculations, and so the doses were quite dissimilar. It was necessary to trace through the sequence of calculations, identifying and correcting differences where they occurred. In following the calculation sequence, several ordered procedures were followed:

(1) From simulation 1 to simulation 3: By far the bulk of the comparisons were run on the first simulation run, in which parameters were given nominal values. The next two simulations were used to provide further tests after agreement was satisfactory on this first simulation. Simulations 4 to 6 were also run to produce more comparison results, but were not used to locate differences.

(2) Following the data flow: Initial comparisons concentrated on the first variables calculated, typically radionuclide concentrations in the tailings source model. These comparisons were possible using intermediate variables that had been printed out in the

reference UTAP2 runs. Later comparisons extended to variables calculated in other components of the tailings model, including dose estimates.

(3) Increasing time: Initial comparisons took place at time 0. Later comparisons applied to time = 1 year, then 2 years, and so on up to 1000 years.

(4) Increasing precision: Initial comparisons looked for gross discrepancies between SYVAC3-UT2 and UTAP2 values. Later comparisons identified discrepancies at the level of 1%, and eventually 0.01%.

Once discrepancies between UTAP2 and SYVAC3-UT2 values were identified, they were investigated in a variety of ways. These included:

(1) Examining calculated variables at earlier times, by backtracking through output files or using a debugger, in an attempt to localize the source of the differences.

(2) Comparison of the SYVAC3-UT2 listings with the specifications, to determine that the code was a correct implementation of the specifications.

(3) Comparison of the specifications with the UTAP2 documentation, in cases where other investigations revealed no explanation of the problem.

(4) Comparison of the specifications (or the SYVAC3-UT2 code) with a listing of the UTAP2 model code when no other explanation of the problem could be found.

These steps describe the general procedure followed, although there were some differences in specific cases. For example, investigation of some discrepancies involved detailed comparisons of input data sets, rather than inspection of code.

In a few other cases, even comparison with the UTAP2 code did not reveal the source of the problem. In such instances, it became important to follow the detailed workings of the UTAP2 code, and to examine the intermediate variable values it produced. Since a working version of UTAP2 was not available, excerpts from UTAP2 were recoded in APL for comparison with SYVAC3-UT2. Though effective at finding the source of discrepancies, this approach was more time-consuming than visual comparisons, and so it was used only after multiple comparisons of specifications and UTAP2 code failed to resolve a difference.

Whatever variations were used, comparison involving direct examination of the UTAP2 code was always the last step in the analysis of the source of a discrepancy. We had originally planned that we would not have access to the UTAP2 code, to ensure that SYVAC3-UT2 was developed totally independently from UTAP2. We had also planned that, when required, any unresolved problems would be forwarded to SENES Consultants for clarification. These plans were changed, however, because of time constraints. It quickly became clear that there were many discrepancies between the specifications and the UTAP2 code, and that each one required a detailed comparison of specifications and code to resolve. It was therefore decided, with the agreement of the Scientific Authority, that UTAP2 code listings would be used when required, so that the comparison project would achieve as much progress as possible within the time available.

Correction of Code and Specifications

When errors were found in the specifications, and/or when additional information required modifications to the specifications, the specifications were changed before the code was revised. This control was taken to ensure that the SYVAC3-UT2 code continued to match the specifications, and to ensure that the specifications were always current.

Specifications that required change because they did not match the documentation on which they were based were simply changed and the error noted. Specifications that required change because the original documentation was incorrect or incomplete or ambiguous were annotated to indicate that the specifications no longer matched the written documentation of UTAP2. In this last case, a suitable reference was made to the source of the information that led to the revision, such as a letter from SENES Consultants, or direct examination of the UTAP2 source code.

Code Optimization

Not all changes to SYVAC3-UT2 were made to correct errors. Some changes were made to make the code run faster. SYVAC3-UT2 initially took about 15 seconds per time-step to execute on a COMPAQ PORTABLE 286 microcomputer. This amount of time was considered excessive. A check was run on the code to identify the time-consuming sections (primarily calculation of pH values, and computation of air concentrations of radionuclides). To reduce the time, two steps were taken:

(1) pH calculations: the bisection method originally used to solve for pH values was replaced by a more sophisticated equation solver, namely the Van Wijngaarden-Dekker-Brent method, as documented in Press et al (1986), somewhat modified for this application. Use of Newton's method, as in UTAP2, was also possible, but use of a completely different method was thought to be a better test of the UTAP2 code.

(2) Moving calculations out of loops: time-consuming computations were moved out of loops, both in pH calculations and in calculations of air concentrations. This change had the largest effect on timings.

One other change was made to match UTAP2 and had the side-effect of speeding up the code. According to the documentation and a clarification by SENES, the pH of the gypsum-enriched zone at each time step was calculated iteratively, along with some other variables, from a set of implicit equations. However it was found from inspection of the UTAP2 code that iteration was not in fact used. Removing it from SYVAC3-UT2 reduced the execution times.

The cumulative effect of all these contributors was to reduce the execution time to less than 6 seconds per time-step. Other code optimization steps are also possible; for example, SYVAC3-UT2 calculates concentrations at all possible locations in the study area, not all of which are required in the final calculation of lake pH and dose to a particular receptor.

3.0 COMPARISON OF UTAP2 AND SYVAC3-UT2

3.1 Comparison Criteria

A major goal of this project is the performance and documentation of a comparison of results from UTAP2 and SYVAC3-UT2. If the two codes were relatively simple, it could be expected that all results would show agreement within a large number of significant figures, and there would be no need for formal comparison criteria. Such agreement was not expected here, however, since the uranium tailings model is very complicated, and it is embedded within the large and complicated executive modules of UTAP2 and SYVAC3-UT2. Furthermore, both UTAP2 and SYVAC3-UT2 are designed to operate in a probabilistic or Monte Carlo fashion, so that exact agreement of all results is not feasible.

These considerations have led to the establishment of a formal set of comparison criteria for the comparison of UTAP2 and SYVAC3-UT2. Prior to the start of the comparison, the Scientific Authority, SENES Consultants and staff from AECL discussed these issues, and developed a set of criteria that would be used to summarize how well the two codes agreed. Criteria were set for both the deterministic and probabilistic simulations. (A deterministic simulation is a single application of the codes, in which all parameter values have known values, whereas probabilistic simulations consist of many applications in which all input parameters are randomly sampled from their probability distribution functions.)

As noted in Section 1.2, the scope of this report has been reduced somewhat, and not all of the criteria were applied. Nevertheless all of the criteria are detailed below since they would be of value for similar projects. Modifications to the criteria, as applied in this report, are also noted below.

Introductory Comments

For both the deterministic and probabilistic cases, the comparison criteria will be applied to the major output variables:

(1) pH of the lake;
(2) dose from the ingestion of vegetables;
(3) dose from the ingestion of caribou and moose;
(4) dose from the ingestion of fish;
(5) dose from the ingestion of water;
(6) dose from the inhalation of dust;
(7) dose from the inhalation of radon gas; and
(8) dose from external groundshine.

Other common elements of the deterministic and probabilistic comparisons are:

(1) UTAP2 simulation results will be supplied by SENES on 5-1/4" floppy disks in the following format: one variable value per line with the variable name and time clearly marked. All numeric values will be recorded to at least five significant figures and will be rounded - off. The data for deterministic runs will contain values for major calculated variables (listed below), in addition to the above eight major output variables, to simplify the process of isolating differences between the codes.
(2) SYVAC3-UT2 results will be produced at WNRE, and will also be available on floppy disks in the same format as the UTAP data.

Deterministic Comparison Criteria

For each deterministic simulation, the seven dose variables and the lake pH will be compared at 11 times: 0, 50, 100, 150, 200, 250, 350, 500, 650, 800, 1000 years. For each variable at each time, an absolute percentage difference between UTAP and SYVAC3 results will be computed, using the formula |UTAP-SYVAC3|/UTAP x 100% (where UTAP and SYVAC3 designate variable values from UTAP2 and SYVAC3-UT3 respectively).

Results will be summarized for each of the eight variables by taking:

(1) the absolute percentage difference at the start of the simulation (t=0 years);
(2) the absolute percentage difference at the end of the simulation (t=1000 years);
(3) the maximum absolute percentage taken over the remaining nine values.

The set of 24 results (eight variables x three statistics per variable) will then be assigned to one of four categories, defined as follows:

"Excellent" agreement: At least 21 of the 24 absolute deviations are within 2%, and all 24 are within 20%.

"Good" agreement: At least 18 of the 24 absolute deviations are within 2%, and all 24 are within 20%.

"Acceptable" agreement: At least 15 of the 24 absolute deviations are within 2%, and all 24 are within 20%.

"Poor" agreement: Any other combination of results.

In all cases, any evidence of systematic differences should be examined in detail.

Six deterministic simulations will be used in the deterministic comparisons. In order of application they are:

(1) Simulation with all sampled parameters fixed at median values.
(2) Simulation with all sampled parameters fixed at their minimum values

(or at the mean minus three standard deviations if there is no minimum value).

(3) Simulation with all sampled parameters fixed at their maximum values (or at the mean plus three standard deviations if there is no maximum value).

(4-6) Simulations with all parameters randomly selected; i.e. any three different randomly-chosen simulations, as chosen by sampling in UTAP2.

The goal is to achieve excellent agreement on all six deterministic simulations. It is anticipated that attaining this goal will require some preliminary comparisons in which poorer agreement will be found. The deterministic simulations will be used one-at-a-time. Comparisons will not be made on the second simulation until excellent or good agreement is reached on the first; not on the third until excellent or good agreement is reached on the first and second; etc. Where differences between SYVAC3-UT3 and UTAP2 are found, the reasons will be identified and changes will be made in SYVAC3-UT3 to make it match UTAP2. A record will be kept of the results of all preliminary comparisons and the changes needed to make the codes match. It is anticipated that the sixth simulation (and possibly earlier ones) will give excellent agreement the first time it is run. This event will be taken as evidence that all the major differences between the codes have been found.

For use in the comparisons of the first three deterministic simulations, the following list of major calculated variables will be used as a starting point:

(1) Solid and aqueous concentrations in layers 1, 2 and 3 of all important chemical species (including PH1, PH2, PH3, WCONC (i,j,t) and CONC (i,j,t); i = 1 to 10, j = 1 to 3, and t is equal to time points specified below).

(2) Aqueous concentrations in layer 4 (including WCONC(i,j,t) and PH4, i = 1 to 10, j = 4, at each of the specified time points).

(3) The total radon gas flux from the tailings (EMRATE(5); at each of the specified time points).

(4) Air concentrations at the critical receptor located in a specified ring and sector (AIRC (i, location); i = 1 to 5, specifying also location, at each of the specified time points).

(5) Concentrations of radionuclides in the three soil layers (SWCONC (i,j); ZTOT (i,j); i = 1 to 4, j = 1 to 3, at each of the specified time points.

(6) Concentrations of radionuclide in the two edible vegetable types at the location of the critical receptor (AVEGC (i, location), BVEGC (i, location); i = 1 to 4, at each of the specified time points).

(7) Discharge concentrations of radionuclides from subsurface transport (GWATC (i,t); i = 1 to 4, at each of the specified time points).

(8) Concentrations and pH at watershed nodes 1 and 2 (assuming that the critical receptor obtains his drinking water from one of these nodes) (WATC (i,n), WATPH (n); i = 1 to 8, n = 1 to 2, at each of the specified time points).

(9) Watershed average concentrations of radionuclides in air and water (WATAVG (i), AIRC (i, n+1), i = 1 to 4, n+1 = number of receptor locations (n) plus 1, at each of the specified time points).

(10) Concentrations of radionuclides in fish flesh (FISHC (i,n), i = 1 to 4, n = location, at each of the specified time points).

(11) The pH and seven doses making up the "major output variables" (at each of the specified time points).

Values for these variables will be provided at the first five time-steps, and at t = 0, 50, 100, 150, 200, 250, 350, 500, 650, 800 and 1000 years. For the median and minimum simulations the time step will be 1 year (16 time-points in total); for the maximum simulation the time step will be 10 years (15 time-points total). Precipitation and wind speed will be fixed; for each time step, at a constant value for the first three deterministic simulations. Any other time-varying parameters should be treated similarly.

Probabilistic Comparison Criteria

For the probabilistic comparisons, two approaches will be followed: two-way analysis of variance, and alternate tests.

(1) Two-Way Analysis of Variance

These comparisons will involve an equal number of simulations (at least 500) from SYVAC-UT3 and UTAP2. The seven dose variables and the lake pH will be compared at the 11 times used in the deterministic comparisons (i.e. 0, 50, 100, 150, 200, 250, 350, 500, 650, 800, and 1000 years). Before the comparisons, each of the eight variables will be transformed if necessary so that the UTAP2 and SYVAC3-UT2 values at each time follow approximate normal distributions as displayed on a probit plot. For example, it is expected that the dose variables will require a log transformation before analysis, since they tend to display lognormal characteristics.

A two-way analysis of variance (ANOVA) will be carried out for each of the eight variables. The transformed data will be classified in two ways, by computer code (SYVAC3-UT2 or UTAP2) and by time (11 values). If 500 runs are carried out using each code, there will be 500 observations for each combination of code and time. Tests of significance will be based on the assumption that each treatment effect (i.e. effects of codes and times) is fixed (reproducible).

The results of the ANOVA analysis will then be assigned, for each of the eight variables, to one of three categories, defined as follows:

"Excellent" agreement: there is no evidence, at the 95% level to reject the hypothesis that UTAP2 and SYVAC3-UT2 produce the same results.

"Good" agreement: there is evidence at the 95% level, but not the 99% level, to reject the hypothesis that UTAP2 and SYVAC3-UT2 produce the same results.

"Poor" agreement: any other result.

A summary of the agreement for all eight variable will also be provided.

(2) Alternate Tests

Several alternate tests will be investigated with the probabilistic simulations, with the objectives being to provide a more thorough and complete comparison, and to devise techniques to present the comparison results in a simplified fashion. The following tests are examples of those that were to be investigated:

(a) Comparison of the upward (or downward) cumulative probabilistic curves of total dose, at t=0 500 and/or 1000 years.

(b) Comparison of the total dose versus time plots.

(c) Comparison of tail probabilities.

Modifications to the Criteria

The reduced scope of this project meant that not all of the above criteria were applied. In particular, it was not possible to complete the probabilistic comparison (due to time constraints) and the corresponding criteria were not used. For the deterministic simulations, the following changes to the criteria were made:

(1) The pH of the lake was redefined to "pH of the lake nearest the tailings site", since the system modelled contained three lakes, and since the first lake is most affected by the tailings.

(2) Dose from external groundshine was not coded in SYVAC3-UT2, due to the late completion of its corresponding specifications. As a consequence, only seven variables (pH of the lake and six dose variables) were compared at 11 times. The requirements for the qualitative summary (excellent, good, acceptable and poor) were also scaled down; for example excellent agreement required that 18 (not 21) of the 21 (and not 24) absolute deviations are within 2%, and all 21 are within 20%.

(3) For the last three (random sample) deterministic simulations, the SENES data did not include dose from ingestion of water. Consequently only six variables were compared at 11 times, and the qualitative summary criteria were scaled as above.

3.2 Comparison of the Deterministic Results

Six deterministic simulations were used in the detailed comparison of UTAP2 and SYVAC3-UT2 results. Of these, two achieved excellent agreement, and one gave good agreement. Achieving these results required a significant amount of work in finding and eliminating discrepancies between the codes. In the end, it was a shortage of time that prevented us from completing the comparison of all six deterministic simulations, and from achieving excellent agreement in all comparisons.

The input parameter values used in the first three simulations are shown in Table 3.2/1. The first deterministic simulation was one in which all parameters were fixed at their "nominal" values. The second and third simulations were ones in which all parameters were fixed at their minimum and maximum allowed values, respectively. The last three simulations were ones in which the parameter values were sampled randomly from their probability distributions.

The six deterministic simulations varied most but not all of the input parameters. In particular, two important parameters were not varied, and consequently some portions of the tailings model were not tested. These two parameters are:

(1) The net precipitation (NPRCP). This parameter was fixed at 0.4 ma^{-1} (and equal to the average net precipitation, AVPRCP). The tailings model and specifications in Appendix B allow that NPRCP could change at each time step, with a value sampled from its probability distribution.

(2) The initial mass fraction of lime ($CaCO_3$) in the tailings (XLIME). This parameter takes on two discrete values, defining the two scenarios where lime has or has not been added to the tailings. The only scenario covered in the six deterministic simulations was the no-lime scenario (XLIME=0.0).

One parameter, the time step size DT, was treated in a special way in these simulations, since UTAP2 imposed some limitations on its value. The only options encountered in the six deterministic simulations were for DT fixed at one year and/or ten years. Furthermore, only two hundred time steps could be used in UTAP2, so a one-year time step could be used only in simulations of two hundred years duration or less. To achieve a thousand year simulation in all three deterministic runs, the following stratagem was used in the first two runs. A time step size of one year was used to yield dose estimates for the first two hundred years. A time step size of ten years was used in a separate simulation to yield dose estimates from two hundred years to one thousand years. In the third run, only the maximum value of DT (i.e. ten years) was used.

For each of the first three simulations, a total of 21 results were compared (not 24 because dose from external groundshine was not coded into SYVAC3-UT2). Tables 3.2/2 to 3.2/4 contain a summary of the final results. Excellent agreement was obtained for the nominal-value simulation and for the maximum-value simulation, and good agreement for the minimum value simulation.

TABLE 3.2/1

VALUES OF PARAMETERS THAT CHANGED BETWEEN DETERMINISTIC RUNS

PARAMETER NAME	FIRST SIMULATION NOMINAL VALUES	SECOND SIMULATION MINIMUM VALUES	THIRD SIMULATION MAXIMUM VALUES
AFACT	1.0	0.5	1.0
AFLOC(01)	0.5	0.1	0.6
AFLOC(02)	0.1	0.0	0.2
BFACT	1.0	0.5	1.0
BFLOC(01)	0.5	0.1	0.6
BFLOC(02)	0.1	0.0	0.2
BIOACF(01)	1.55E-6	1.0E-8	5.8E-5
BIOACF(02)	11.8E-6	1.1E-6	1.1E-4
BIOACF(03)	17.4E-6	1.7E-6	5.7E-4
BIOACF(04)	13.1E-6	1.2E-6	6.0E-4
BURYF	.6	0.5	.7
CARMIN(02)	3.2E3	0.0	3.2E3
CFLOC(01)	0.5	0.0	1.0
CFLOC(02)	0.5	0.0	1.0
CLEADI	2.0	1.0	3.0
CURRNT	17.325E4	3.15E4	3.15E5
DCGWAT(01)	.02	5.E-3	.5
DCGWAT(02)	.5	0.05	5.0
DCGWAT(03)	.67	0.13	3.5
DCGWAT(04)	.07	0.01	0.5
DEPVEL	.02	3.0E-3	3.0E-2
DMIX	1.5	1.0	2.0
DUNSAT	1.0	0.75	1.25
DUREXP(01)	5.184E6	2.6E6	7.8E6
DUREXP(02)	5.184E6	2.6E6	7.8E6
DUREXP(03)	2.592E6	1.3E6	3.9E6
DUREXP(04)	2.592E6	1.3E6	3.9E6
EFR	0.5	0.2	0.8
EMANAT	0.2	2.0E-2	0.9
FACTCO	.4	0.3	.5
FAIBM	.9	0.8	.95
FAILC	.4	0.05	.5
FAISFC	.4	0.05	.5
FDEPED(01)	1.0	0.8	1.0
FDEPED(02)	0.1	0.05	0.15
FDEPED(03)	1.0	0.8	1.0
FDEPED(04)	1.0	0.8	1.0
FDEPED(05)	1.0	0.8	1.0
FDEPSF(01)	0.2	0.1	0.3
FDEPSF(02)	0.2	0.1	0.3
FDEPSF(03)	0.2	0.01	1.0
FDEPSF(04)	0.2	0.01	1.0
FDEPSF(05)	0.95	0.8	1.0
FFLOC(02)	0.05	0.0	0.10
FIRC	7.0E3	5.0E3	9.0E3
FLEAD	0.95	0.92	0.98
FMTCC(01)	3.4E-7	1.1E-7	1.0E-6
FMTCC(02)	2.0E-7	0.7E-7	6.0E-7

TABLE 3.2/1 (Continued)

VALUES OF PARAMETERS THAT CHANGED BETWEEN DETERMINISTIC RUNS

PARAMETER NAME	FIRST SIMULATION NOMINAL VALUES	SECOND SIMULATION MINIMUM VALUES	THIRD SIMULATION MAXIMUM VALUES
FMTCC(03)	4.0E-7	1.3E-7	12.0E-7
FMTCC(04)	5.1E-7	1.7E-7	15.0E-7
FMTCM(01)	3.4E-7	1.1E-7	1.0E-6
FMTCM(02)	2.0E-7	0.7E-7	6.0E-7
FMTCM(03)	4.0E-7	1.3E-7	12.0E-7
FMTCM(04)	5.1E-7	1.7E-7	15.0E-7
FNPRCP	1.5E-1	0.07	0.3
FPREC	1.23E2	8.4E1	1.56E2
FRACGP	5.5E-2	5.0E-2	6.0E-2
FRACTH	0.3	0.2	0.4
FRACU	0.6	0.3	0.9
FRAD	0.6	0.25	0.95
FT230	0.95	0.92	0.98
FT232	0.65	0.60	0.70
FURAN	0.95	0.92	0.98
FWAT	.16	0.02	.48
HSRC	2.0	1.0	3.0
INOCC(01)	0.75	0.50	0.90
INOCC(02)	0.75	0.50	0.90
KDLEAD	60.0E-6	20.0E-6	100.0E-6
KDPRIM	2.0E-02	2.0E-03	3.0E-01
KDRAD	40.0E-6	5.0E-6	75.0E-6
KDUO2	3.0E-5	1.1E-6	8.1E-4
KPRIME	5.0E-2	2.0E-2	2.5E-1
KRAD	0.53	0.50	0.56
MNPRCP	0.4	0.15	0.65
MOMIN(02)	3.2E3	0.0	3.2E3
MPCH2O	1.5E1	5.0	2.5E1
O2DIFF	7.0E1	3.0E1	13.0E1
OF(01)	0.6	0.4	0.9
OF(02)	0.9	0.8	1.0
PCTHOR	0.03	0.02	0.04
POGWAT	0.33	0.30	0.36
POROS	4.0E-1	3.5E-1	4.5E-1
PYRITI	700.0	600.0	800.0
RHOS(01)	1.29E2	2.0E1	4.50E2
RHOS(02)	1.342E3	1.0E3	1.800E3
RHOTAL	1.4E6	1.1E6	1.7E6
RRAIN	8.12E1	6.5E1	9.75E1
RSOIL	5.50E-8	1.00E-8	1.00E-7
SGGWAT	2650.0	2320.0	2980.0
SILT	4.5E1	1.0E1	9.0E1
SOILKD(01)	3.2E-1	1.3E-4	7.9E2
SOILKD(02)	0.7	3.3E-3	1.5E2
SOILKD(03)	3.4	1.8E-1	6.3E1
SOILKD(04)	2.2	5.1E-3	9.5E2
SPTC(01,01)	6.08E-4	7.67E-6	7.00E-3
SPTC(02,01)	4.20E-3	5.19E-5	3.40E-1
SPTC(03,01)	4.0E-3	4.94E-5	3.24E-1

TABLE 3.2/1 (Concluded)

VALUES OF PARAMETERS THAT CHANGED BETWEEN DETERMINISTIC RUNS

PARAMETER NAME	FIRST SIMULATION NOMINAL VALUES	SECOND SIMULATION MINIMUM VALUES	THIRD SIMULATION MAXIMUM VALUES
SPTC(04,01)	8.47E-3	8.03E-5	8.93E-1
SPTC(01,02)	3.17E-4	2.06E-5	4.89E-3
SPTC(02,02)	4.20E-3	2.62E-4	6.72E-2
SPTC(03,02)	4.00E-3	2.50E-4	6.40E-2
SPTC(04,02)	2.65E-3	1.29E-4	6.60E-2
SPTC(01,03)	6.6E-3	8.31E-5	5.24E-1
SPTC(02,03)	2.23E-2	2.47E-4	2.01E00
SPTC(03,03)	2.16E-2	1.71E-3	2.71E-1
SPTC(04,03)	2.11E-1	1.87E-3	2.39E-1
SPTC(01,04)	6.6E-3	8.31E-5	5.24E-1
SPTC(02,04)	2.23E-2	2.47E-4	2.01E00
SPTC(03,04)	2.16E-2	1.71E-3	2.71E-1
SPTC(04,04)	2.11E-1	1.87E-3	2.39E-1
STORM	42.0	36.0	48.0
SULPRD	1.4E-6	0.4E-6	4.2E-6
THALF	1.5E1	1.0E1	2.0E1
VEGLAM(01)	5.73E-7	2.9E-7	1.2E-6
VEGLAM(02)	5.73E-7	2.9E-7	1.2E-6
VEGLAM(03)	5.73E-7	2.9E-7	1.2E-6
VEGLAM(04)	5.73E-7	2.9E-7	1.2E-6
VEGLAM(05)	2.19E-9	1.5E-9	4.40E-9
WATEPS	0.94	0.83	0.97
WATVTC(01)	1.5E-5	1.0E-6	7.0E-4
WATVTC(02)	1.1E-5	1.0E-6	1.6E-4
WATVTC(03)	1.3E-4	4.0E-5	4.3E-4
WATVTC(04)	4.5E-5	1.0E-5	3.3E-4
WC(01)	1.08	0.75	1.4
WC(02)	1.30E-1	0.05	0.36
WFLOC(01)	0.6	0.4	0.9
WFLOC(02)	0.9	0.8	1.0
WIRC	11.5E-3	7.7E-3	15.3E-3
WIRM	0.036	0.024	0.048
WKDPB	1.5E-2	1.0E-3	2.3E-1
WKDRA	6.5E-3	0.4E-3	1.0E-1
WKDU	4.5E-3	0.4E-3	4.8E-2
WSIGS(02)	230.	95.	615.
WSIGS(04)	260.	105.	765.
WSIGS(07)	210.	85.	515.
WTSFLX	2.0E-2	2.0E-3	2.0E-1
XRADI	3.5E-6	2.5E-6	4.5E-6
XRGWAT	35.	25.	200.
YDEN(01)	2.0E3	1.0E3	3.0E3
YDEN(02)	2.0E3	1.0E3	3.0E3
YDEN(03)	7.5E2	5.0E2	1.0E3
YDEN(04)	7.5E2	5.0E2	1.0E3
YDEN(05)	5.0E2	4.0E2	6.0E2

TABLE 3.2/2

COMPARISON OF UTAP2 AND SYVAC3-UT2 RESULTS FOR DETERMINISTIC RUN NUMBER 1 (NOMINAL VALUES)*

UTAP2 RESULTS

TIME	WATPH[2]	WATD	INHD	RADD	VEGD	FISHD	MEATD
0.	4.1446	367.11	0.676796	0.208520	0.108881	21.6213	1.3794
50.	4.1808	192.55	0.072373	0.125380	0.111888	11.7453	0.7471
100.	4.5149	153.85	0.062701	0.122160	0.133419	14.4532	0.5921
150.	6.9391	144.94	0.062314	0.118390	0.141281	51.5272	0.5609
200.	7.1845	143.92	0.062100	0.112650	0.146014	51.1554	0.5538
250.	7.2361	149.95	0.061913	0.105200	0.150687	52.9257	0.5689
350.	7.2570	62.90	0.006168	0.076127	0.054620	18.4210	0.1431
500.	7.2590	178.31	0.006136	0.072008	0.047384	53.4004	0.4151
600.	7.2591	227.68	0.006106	0.068149	0.041769	68.4065	0.5323
800.	7.2591	169.55	0.006078	0.064532	0.037188	51.1640	0.4009
1000.	7.2591	61.70	0.006044	0.060061	0.032290	18.6117	0.1466

SYVAC3-UT2 RESULTS

TIME	WATPH[2]	WATD	INHD	RADD	VEGD	FISHD	MEATD
0.	4.1447	367.11	0.676796	0.208518	0.108882	21.6244	1.3791
50.	4.1808	192.58	0.072492	0.125385	0.111885	11.7477	0.7469
100.	4.5149	153.86	0.062701	0.122160	0.133425	14.4535	0.5919
150.	6.9391	144.95	0.062314	0.118389	0.141287	51.5304	0.5606
200.	7.1845	143.93	0.062101	0.112652	0.146019	51.1590	0.5535
250.	7.2361	149.80	0.061903	0.105071	0.150489	52.8671	0.5678
350.	7.2570	62.96	0.006167	0.076005	0.054563	18.4457	0.1430
500.	7.2590	178.38	0.006135	0.071894	0.047331	53.4277	0.4149
650.	7.2591	227.78	0.006105	0.068042	0.041720	68.4492	0.5323
800.	7.2591	169.72	0.006078	0.064432	0.037143	51.2301	0.4013
1000.	7.2591	61.90	0.006043	0.059969	0.032250	18.6903	0.1472

DIFFERENCE IN PERCENT

TIME	WATPH[2]	WATD	INHD	RADD	VEGD	FISHD	MEATD
0.	0.00	0.00	0.00	0.00	0.00	0.01	-0.02
50.	0.00	0.02	0.16	0.00	0.00	0.02	-0.03
100.	0.00	0.01	0.00	0.00	0.00	0.00	-0.04
150.	0.00	0.01	0.00	0.00	0.00	0.01	-0.05
200.	0.00	0.01	0.00	0.00	0.00	0.01	-0.06
250.	0.00	-0.10	-0.02	-0.12	-0.13	-0.11	-0.19
350.	0.00	0.10	-0.01	-0.16	-0.11	0.13	-0.08
500.	0.00	0.04	-0.01	-0.16	-0.11	0.05	-0.03
600.	0.00	0.05	-0.01	-0.16	-0.12	0.06	0.00
800.	0.00	0.10	-0.01	-0.16	-0.12	0.13	0.09
1000.	0.00	0.33	-0.01	-0.15	-0.13	0.42	0.39

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* Units are years for TIME, pH units for WATPH[Z] and μSv/a for all others.

TABLE 3.2/3

COMPARISON OF UTAP2 AND SYVAC3-UT2 RESULTS FOR DETERMINISTIC RUN NUMBER 2 (MINIMUM VALUES)*

UTAP2 RESULTS

TIME	WATPH[2]	WATD	INHD	RADD	VEGD	FISHD	MEATD
0.	4.4466	307.96	0.086139	0.006119	0.000377	3.9747	0.4324
50.	4.1729	315.44	0.012562	0.001847	0.000602	2.6991	0.3192
100.	4.2810	234.24	0.012527	0.002003	0.000680	2.3678	0.2506
150.	4.4258	222.54	0.012413	0.002180	0.000685	2.6827	0.2394
200.	4.7005	218.15	0.012319	0.002394	0.000675	5.1325	0.2349
250.	6.5682	224.25	0.012239	0.002664	0.000660	11.7544	0.2427
350.	7.1119	223.21	0.012137	0.003412	0.000636	11.6210	0.2375
500.	7.2112	257.97	0.012024	0.003846	0.000602	12.8118	0.2466
600.	7.2255	186.28	0.001193	0.003635	0.000057	8.0086	0.1227
800.	7.2278	92.97	0.001183	0.003437	0.000054	4.1340	0.0671
1000.	7.2282	4.71	0.001172	0.003193	0.000050	0.1893	0.0026

SYVAC3-UT2 RESULTS

TIME	WATPH[2]	WATD	INHD	RADD	VEGD	FISHD	MEATD
0.	4.4466	307.96	0.086139	0.006119	0.000377	3.9747	0.4324
50.	4.1729	315.45	0.012575	0.001847	0.000603	2.6993	0.3192
100.	4.2811	234.24	0.012527	0.002002	0.000680	2.3679	0.2506
150.	4.4258	222.55	0.012413	0.002179	0.000685	2.6829	0.2395
200.	4.7007	218.16	0.012319	0.002394	0.000675	5.1355	0.2349
250.	6.5682	224.07	0.012237	0.002659	0.000659	11.7446	0.2425
350.	7.1119	223.03	0.012135	0.003407	0.000636	11.6119	0.2374
500.	7.2111	276.44	0.012022	0.003842	0.000602	13.7876	0.2672
650.	7.2255	186.50	0.001192	0.003631	0.000057	8.0209	0.1230
800.	7.2278	93.43	0.001183	0.003434	0.000054	4.1600	0.0677
1000.	7.2282	5.13	0.001172	0.003190	0.000050	0.2126	0.0031

DIFFERENCE IN PERCENT

TIME	WATPH[2]	WATD	INHD	RADD	VEGD	FISHD	MEATD
0.	0.00	0.00	0.00	0.00	0.00	0.00	0.00
50.	0.00	0.01	0.10	0.00	0.01	0.01	0.00
100.	0.00	0.00	0.00	0.00	0.00	0.00	0.00
150.	0.00	0.01	0.00	0.00	0.00	0.01	0.00
200.	0.00	0.00	0.00	0.00	0.00	0.06	0.01
250.	0.00	-0.08	-0.02	-0.17	-0.10	-0.08	-0.09
350.	0.00	-0.08	-0.02	-0.13	-0.10	-0.08	-0.08
500.	0.00	7.16	-0.01	-0.10	-0.10	7.62	8.33
600.	0.00	0.12	-0.01	-0.10	-0.10	0.15	0.22
800.	0.00	0.49	-0.01	-0.10	-0.10	0.63	0.85
1000.	0.00	8.92	-0.01	-0.10	-0.10	12.34	19.29

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* Units are years for TIME, pH units for WATPH[Z] and μSv/a for all others.

TABLE 3.2/4

COMPARISON OF UTAP2 AND SYVAC3-UT2 RESULTS FOR DETERMINISTIC RUN NUMBER 3 (MAXIMUM VALUES)*

UTAP2 RESULTS

TIME	WATPH[2]	WATD	INHD	RADD	VEGD	FISHD	MEATD
0.	3.9945	1240.01	2.486955	0.916650	0.189272	325.0464	5.2434
50.	4.2016	22.38	0.363491	0.602280	0.053873	28.5888	0.5173
100.	6.7127	6.48	0.136776	0.304810	0.067245	54.0130	0.1809
150.	7.2184	4.36	0.136590	0.101940	0.087599	36.1915	0.1252
200.	7.2641	6.69	0.114815	0.061452	0.102548	57.3190	0.1552
250.	7.2709	10.33	0.020298	0.059723	0.098741	90.6983	0.1774
350.	7.2722	8.69	0.013642	0.058060	0.138459	76.0490	0.1506
500.	7.2722	32.11	0.013633	0.055698	0.201282	283.9517	0.5458
650.	7.2722	55.88	0.013623	0.053484	0.263293	494.7972	0.9484
800.	7.2722	68.88	0.013615	0.051409	0.324381	610.1645	1.1689
1000.	7.2722	76.18	0.013604	0.048844	0.404472	674.9289	1.2927

SYVAC3-UT2 RESULTS

TIME	WATPH[2]	WATD	INHD	RADD	VEGD	FISHD	MEATD
0.	3.9945	1240.00	2.486985	0.916652	0.189270	325.0909	5.2398
50.	4.2016	22.38	0.363504	0.602283	0.053874	28.5892	0.5168
100.	6.7127	6.48	0.136774	0.304771	0.067231	54.0038	0.1805
150.	7.2184	4.36	0.136588	0.101899	0.087582	36.1805	0.1248
200.	7.2640	6.69	0.114811	0.061414	0.102532	57.3179	0.1548
250.	7.2709	10.33	0.020298	0.059685	0.098737	90.6988	0.1771
350.	7.2722	8.69	0.013642	0.058025	0.138452	76.0494	0.1502
500.	7.2722	32.11	0.013632	0.055664	0.201280	283.9477	0.5452
650.	7.2722	55.88	0.013623	0.053452	0.263286	494.7948	0.9475
800.	7.2722	68.88	0.013615	0.051379	0.324381	610.1545	1.1677
1000.	7.2722	76.18	0.013604	0.048817	0.404462	674.9277	1.2914

DIFFERENCE IN PERCENT

TIME	WATPH[2]	WATD	INHD	RADD	VEGD	FISHD	MEATD
0.	0.00	0.00	0.00	0.00	0.00	0.01	-0.07
50.	0.00	0.00	0.00	0.00	0.00	0.00	-0.09
100.	0.00	-0.02	0.00	-0.01	-0.02	-0.02	-0.23
150.	0.00	-0.03	0.00	-0.04	-0.02	-0.03	-0.36
200.	0.00	0.00	0.00	-0.06	-0.02	0.00	-0.27
250.	0.00	0.00	0.00	-0.06	0.00	0.00	-0.16
350.	0.00	0.00	0.00	-0.06	-0.01	0.00	-0.24
500.	0.00	0.00	0.00	-0.06	0.00	0.00	-0.12
650.	0.00	0.00	0.00	-0.06	0.00	0.00	-0.09
800.	0.00	0.00	0.00	-0.06	0.00	0.00	-0.09
1000.	0.00	0.00	0.00	-0.06	0.00	0.00	-0.10

* Units are years for TIME, pH units for WATPH[Z] and μSv/a for all others.

For each of the last three simulations, a total of 18 results were compared (dose from ingestion of water was also not considered, since the corresponding data was missing from the SENES results). Tables 3.2/5 to 3.2/7 contain a summary of the final results. Excellent agreement was obtained for all three of these simulations.

Nominal Value Simulation

Most of the detailed comparisons of the results from UTAP2 and SYVAC3-UT2 were performed on the first deterministic simulation, in which all parameters were fixed at their "nominal" values, instead of their median values as expected (see Section 3.2). In most cases, a nominal value was equivalent to the mean value of the parameter's probability distribution function, but in some cases it represented another value somewhere within the allowed range of values.

Eventually excellent agreement was obtained on the nominal-value simulation, but in the process we estimate that the simulation was run on SYVAC3-UT2 more than fifty times to identify, locate and correct most of the major differences between the two codes. Most of the comments in item 21 of Appendix A were deduced during this phase of the comparison. The final differences between the two codes for the nominal value simulation were less than 0.5% for all variables at all times.

During the analysis of the nominal-value simulation, several aspects of the project were observed to have a direct effect on the ease with which differences between the codes could be identified. These aspects, which should be considered in planning any future work of this type, include the following:

(1) Detailed output: SENES provided output for each deterministic simulation that included both the major output variables of the simulation as well as many intermediate variables. We found that the detailed output was instrumental in localizing many of the differences. Consider, for example, the following sequence of calculations:

TAILINGS EMISSION RATE OF RADIONUCLIDE, used to calculate
AIR CONCENTRATION OF RADIONUCLIDE, used to calculate
INHALED DOSE FROM RADIONUCLIDE, used to calculate
TOTAL INHALED DOSE

If both the inhaled dose and the air concentrations from which it is calculated differ between the two codes, then one can hypothesize that there is a difference between the codes somewhere in the calculation of air concentrations. If in turn the soil emission rates agree, then the discrepancy has been localized to the intervening code. The size of the section of the code that must be searched for discrepancies has a direct effect on the length of time it takes to find the problem. For this reason, having more intermediate results would reduce the time taken to achieve code agreement. In the ideal situation, the two codes would be running on computers or terminals side by side, and each variable could be checked with a debugger as its value changed.

TABLE 3.2/5
COMPARISON OF UTAP2 AND SYVAC3-UT2 RESULTS FOR DETERMINISTIC RUN NUMBER 4 (RANDOMLY-SAMPLED VALUES)*

UTAP2 RESULTS

TIME	WATPH[2]	WATD	INHD	RADD	VEGD	FISHD	MEATD
0.	3.9912	0.00	1.158997	0.522250	0.026782	58.8673	1.1567
50.	4.1185	0.00	0.202816	0.273260	0.030531	45.1966	0.6026
100.	4.3868	0.00	0.065635	0.279430	0.034213	60.4488	0.5223
150.	6.7625	0.00	0.064979	0.290470	0.035189	265.7518	0.4961
200.	7.1644	0.00	0.064619	0.307140	0.034876	263.4100	0.4921
250.	7.2325	0.00	0.064362	0.329000	0.034270	258.7208	0.4986
350.	7.2546	0.00	0.006393	0.235250	0.004275	41.4221	0.2067
500.	7.2564	0.00	0.006334	0.221140	0.003120	106.6373	0.4951
650.	7.2564	0.00	0.006278	0.207910	0.002923	65.3591	0.2875
800.	7.2564	0.00	0.006227	0.195520	0.002754	22.5393	0.1006
1000.	7.2564	0.00	0.006163	0.180200	0.002545	5.6706	0.0271

SYVAC3-UT2 RESULTS

TIME	WATPH[2]	WATD	INHD	RADD	VEGD	FISHD	MEATD
0.	3.9914	1502.46	1.158980	0.522252	0.026782	58.8889	1.1551
50.	4.1185	342.20	0.202760	0.273257	0.030531	45.1949	0.6019
100.	4.3868	285.83	0.065632	0.279355	0.034208	60.4417	0.5218
150.	6.7624	274.45	0.064976	0.290405	0.035181	265.7396	0.4956
200.	7.1644	274.30	0.064616	0.307068	0.034867	263.4321	0.4917
250.	7.2325	280.28	0.064359	0.328934	0.034261	258.7699	0.4982
350.	7.2546	142.41	0.006393	0.235187	0.004274	41.5839	0.2067
500.	7.2564	344.09	0.006334	0.221078	0.003119	106.8317	0.4949
650.	7.2564	199.79	0.006278	0.207856	0.002923	65.6938	0.2877
800.	7.2564	69.40	0.006226	0.195466	0.002753	22.9963	0.1012
1000.	7.2564	18.19	0.006162	0.180149	0.002544	6.1255	0.0277

DIFFERENCE IN PERCENT

TIME	WATPH[2]	WATD	INHD	RADD	VEGD	FISHD	MEATD
0.	0.01	0.00	0.00	0.00	0.00	0.04	-0.14
50.	0.00	0.00	-0.03	0.00	0.00	0.00	-0.11
100.	0.00	0.00	0.00	-0.03	-0.02	-0.01	-0.09
150.	0.00	0.00	0.00	-0.02	-0.02	0.00	-0.09
200.	0.00	0.00	0.00	-0.02	-0.02	0.01	-0.08
250.	0.00	0.00	0.00	-0.02	-0.03	0.02	-0.07
350.	0.00	0.00	0.00	-0.03	-0.03	0.39	0.02
500.	0.00	0.00	0.00	-0.03	-0.02	0.18	-0.04
650.	0.00	0.00	0.00	-0.03	-0.02	0.51	0.08
800.	0.00	0.00	0.00	-0.03	-0.02	2.03	0.57
1000.	0.00	0.00	0.00	-0.03	-0.03	8.02	2.41

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* Units are years for TIME, pH units for WATPH[Z] and µSv/a for all others.

TABLE 3.2/6
COMPARISON OF UTAP2 AND SYVAC3-UT2 RESULTS FOR DETERMINISTIC RUN NUMBER 5 (RANDOMLY-SAMPLED VALUES)*

UTAP2 RESULTS

TIME	WATPH[2]	WATD	INHD	RADD	VEGD	FISHD	MEATD
0.	3.9834	0.00	0.797211	0.286640	0.055693	49.6456	0.9362
50.	4.1602	0.00	0.192554	0.169660	0.064237	44.3104	0.7985
100.	4.9977	0.00	0.069002	0.167880	0.073202	204.5332	0.8218
150.	7.1658	0.00	0.068893	0.165660	0.075415	271.7397	0.8170
200.	7.2387	0.00	0.068750	0.162510	0.074901	243.0133	0.7327
250.	7.2493	0.00	0.006860	0.157360	0.018067	2.3752	0.0185
350.	7.2512	0.00	0.006831	0.110710	0.010478	1.4097	0.0183
500.	7.2513	0.00	0.006789	0.104550	0.008903	1.2458	0.0162
650.	7.2513	0.00	0.006749	0.098774	0.007953	4.2601	0.0476
800.	7.2513	0.00	0.006712	0.093363	0.007210	10.0354	0.1008
1000.	7.2513	0.00	0.006667	0.086674	0.006442	14.4139	0.1407

SYVAC3-UT2 RESULTS

TIME	WATPH[2]	WATD	INHD	RADD	VEGD	FISHD	MEATD
0.	3.9834	974.30	0.797214	0.286635	0.055694	49.6458	0.9357
50.	4.1605	217.96	0.192589	0.169662	0.064238	44.3260	0.7980
100.	4.9977	189.06	0.068996	0.167760	0.073168	204.4370	0.8209
150.	7.1658	186.47	0.068885	0.165542	0.075355	271.5147	0.8158
200.	7.2387	183.62	0.068743	0.162396	0.074835	267.0644	0.8028
250.	7.2493	9.13	0.006859	0.157239	0.018054	2.4423	0.0186
350.	7.2512	10.02	0.006830	0.110598	0.010471	1.4992	0.0184
500.	7.2513	8.77	0.006788	0.104444	0.008896	1.3471	0.0163
650.	7.2513	32.11	0.006749	0.098676	0.007947	4.3638	0.0478
800.	7.2513	70.38	0.006712	0.093272	0.007204	10.1412	0.1009
1000.	7.2513	99.20	0.006666	0.086590	0.006437	14.5583	0.1409

DIFFERENCE IN PERCENT

TIME	WATPH[2]	WATD	INHD	RADD	VEGD	FISHD	MEATD
0.	0.00	0.00	0.00	0.00	0.00	0.00	-0.05
50.	0.01	0.00	0.02	0.00	0.00	0.04	-0.06
100.	0.00	0.00	-0.01	-0.07	-0.05	-0.05	-0.12
150.	0.00	0.00	-0.01	-0.07	-0.08	-0.08	-0.15
200.	0.00	0.00	-0.01	-0.07	-0.09	9.90	9.57
250.	0.00	0.00	-0.01	-0.08	-0.07	2.82	0.35
350.	0.00	0.00	-0.01	-0.10	-0.07	6.35	0.78
500.	0.00	0.00	-0.01	-0.10	-0.07	8.13	1.07
650.	0.00	0.00	-0.01	-0.10	-0.07	2.43	0.33
800.	0.00	0.00	-0.01	-0.10	-0.07	1.05	0.12
1000.	0.00	0.00	-0.01	-0.10	-0.08	1.00	0.13

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* Units are years for TIME, pH units for WATPH[Z] and μSv/a for all others.

TABLE 3.2/7
COMPARISON OF UTAP2 AND SYVAC3-UT2 RESULTS FOR DETERMINISTIC RUN NUMBER 6 (RANDOMLY-SAMPLED VALUES)*

UTAP2 RESULTS

TIME	WATPH[2]	WATD	INHD	RADD	VEGD	FISHD	MEATD
0.	4.0295	0.00	0.581887	0.436330	0.020177	320.7112	3.7490
50.	4.1781	0.00	0.055513	0.210280	0.025144	107.0171	1.6045
100.	4.5695	0.00	0.048391	0.221380	0.029144	152.5430	1.2491
150.	7.0179	0.00	0.048220	0.235180	0.030392	445.8241	1.1765
200.	7.2055	0.00	0.048076	0.246310	0.031108	432.2227	1.1538
250.	7.2453	0.00	0.047949	0.250110	0.031760	381.9962	1.0558
350.	7.2583	0.00	0.004772	0.221590	0.010092	12.4042	0.1911
500.	7.2593	0.00	0.004739	0.208580	0.012998	45.9173	0.5722
650.	7.2593	0.00	0.004708	0.196380	0.015971	60.1581	0.7183
800.	7.2593	0.00	0.004680	0.184950	0.018765	45.7793	0.4913
1000.	7.2593	0.00	0.004644	0.170820	0.022234	15.3906	0.1645

SYVAC3-UT2 RESULTS

TIME	WATPH[2]	WATD	INHD	RADD	VEGD	FISHD	MEATD
0.	4.0296	836.52	0.581889	0.436332	0.020177	320.7176	3.7488
50.	4.1782	149.91	0.055606	0.210283	0.025144	107.0346	1.6043
100.	4.5695	119.67	0.048385	0.221096	0.029118	152.4290	1.2478
150.	7.0179	112.54	0.048213	0.234898	0.030362	445.3567	1.1751
200.	7.2055	111.84	0.048069	0.246037	0.031078	431.7522	1.1523
250.	7.2452	116.73	0.047942	0.249839	0.031731	422.4732	1.1609
350.	7.2583	39.70	0.004771	0.221333	0.010089	12.4290	0.1912
500.	7.2593	115.68	0.004738	0.208334	0.012996	45.9430	0.5722
650.	7.2593	144.38	0.004708	0.196153	0.015970	60.1913	0.7184
800.	7.2593	97.22	0.004679	0.184738	0.018764	45.8235	0.4914
1000.	7.2593	32.51	0.004644	0.170627	0.022233	15.4371	0.1646

DIFFERENCE IN PERCENT

TIME	WATPH[2]	WATD	INHD	RADD	VEGD	FISHD	MEATD
0.	0.00	0.00	0.00	0.00	0.00	0.00	0.00
50.	0.00	0.00	0.17	0.00	0.00	0.02	-0.01
100.	0.00	0.00	-0.01	-0.13	-0.09	-0.07	-0.10
150.	0.00	0.00	-0.01	-0.12	-0.10	-0.10	-0.12
200.	0.00	0.00	-0.01	-0.11	-0.10	-0.11	-0.12
250.	0.00	0.00	-0.01	-0.11	-0.09	10.60	9.95
350.	0.00	0.00	-0.01	-0.12	-0.02	0.20	0.02
500.	0.00	0.00	-0.01	-0.12	-0.02	0.06	0.00
650.	0.00	0.00	-0.01	-0.12	-0.01	0.06	0.01
800.	0.00	0.00	-0.01	-0.11	-0.01	0.10	0.01
1000.	0.00	0.00	-0.01	-0.11	0.00	0.30	0.06

* Units are years for TIME, pH units for WATPH[Z] and µSv/a for all others.

(2) UTAP2 code listing: To speed up the identification of the cause of the differences, SENES also provided a listing of the portions of UTAP2 containing the uranium tailings model (with the agreement of the Scientific Authority). We found that this listing was very useful in tracking down many of the differences. To ensure that SYVAC3-UT2 was developed independently of UTAP2, we did not access the UTAP2 listing until SYVAC3-UT2 was coded and the detailed comparisons had begun. In tracking down differences, we also adopted the strategy that the UTAP2 listing would not be examined until other avenues had been exhausted, including the checking of the SYVAC3-UT2 code against its specifications and the checking of the specifications against the SENES documentation. (Also, in most instances, one person examined the UTAP2 listing, and a different person modified SYVAC3-UT2, to help ensure that modifications were developed independently from UTAP2).

(3) Precision of variables: The comparison criteria included the specification of five significant figures for all variables involved in the comparisons. Unfortunately we did not take into account that some variables were calculated iteratively to a preset precision. For example, the pH of layer 2 (PH2) in the tailings pile was calculated iteratively by UTAP2 to a precision of 0.01 pH units. SYVAC3-UT2 used a different algorithm to calculate PH2, and it also iterated until successive values of PH2 differed by less than 0.01 pH units. Consequently differences in the fourth and fifth significant figures of PH2 were difficult to interpret. They could have been due to lack of precision in convergence, or they could have been due to differences between the two codes. Since the pH values of the tailings layers play an important role in the calculation of many other variables, slight variations in the calculations of pH could have significant effects elsewhere in the comparisons. This problem was resolved when a special run of UTAP2 with a tighter tolerance on the pH iterations showed that the original calculations were in fact correct to four decimal places. The convergence criterion in SYVAC3-UT2 was then tightened to 0.0001 pH units, allowing comparisons to all five significant figures (it was assumed that all other results from UTAP2 were also accurate to within 0.0001 pH units).

(4) Model discontinuities: The uranium tailings model included several physical and chemical discontinuities, where the behaviour of some aspect of the system changed abruptly with time. Many variables in the tailings pile, for example, were described using different equations depending on whether or not gypsum was present in a particular layer. Since the gradual depletion of gypsum was determined through a series of complex calculations, UTAP2 and SYVAC3-UT2 could arrive at slightly different times for the complete depletion of gypsum in a tailings layer. It was possible, with a step-size of 10 years, that UTAP2 and SYVAC3-UT2 could differ by as much as 10 years in calculating the time of gypsum depletion. Consequently there could be significant differences between the codes for a variable at particular values of time where such discontinuities existed.

These differences could persist throughout the simulation for those variables that were calculated using a finite-difference equation, since a difference occurring at one time would be propagated through later calculations.

(5) Stability of computation: Some of the computations in the uranium tailings model were sensitive to very small differences in values of some variables. For example, the concentration of iron (II) in the aqueous phase at the bottom of the unsaturated zone was calculated using an equation with differences of powers of PH2, the pH of that layer. Small differences in PH2 were magnified to larger differences in the concentration of iron. On the other hand, some calculations were extremely tolerant of differences in input variable values. For example, the calculation of pH in a lake was quite insensitive to the concentration of sulphate ions in the mixing layer in the tailings, on which it depended. Differences of orders of magnitude in the concentration could yield differences in pH in the third or fourth decimal place. These two types of behaviour made it difficult to identify significant differences between the two codes.

Our investigations during the comparisons with the nominal value simulation also led to one observation that may indicate further refinement in the model is needed: the calculated results depend on the time step-size, DT, used in the simulations and in particular calculated results are different at t=0 for DT=1 and DT=10 years. From SYVAC3-UT2 results, it was clear that doses calculated at 0, 50, 100, 150 and 200 years differed depending on whether a one-year or a ten-year time step was used. For example, the dose from drinking water at 0 years was 1240 μSv/a with a one-year time step, versus 819 μSv/a with a ten-year time step. The same conclusion holds for UTAP2, since UTAP2 and SYVAC3-UT2 produced the same sequence of results from 0 to 1000 years, each using one-year time steps for results up until 200 years, and ten-year time steps to get the later results. The reasons for the differences at 0 years became apparent when we re-examined the specifications - some initial conditions depended on DT. At later times, the differences may have been due to residual effects of the initial conditions (or it could be due to convergence problems with the finite difference equations; this possible problem should be addressed in the UTAP2 documentation).

The observation that DT affects dose estimates directly was unexpected, particularly at t=0, since the usual practice in simulations of this type is that value(s) of DT are chosen that do not affect the results. It may be an indication that the initial conditions have not yet been fully integrated with the overall tailings model. In any case, the discussion of the initial conditions (see, for example, pp 3-2 of SENES (1986)) needs further clarification.

Minimum Value Simulation

As noted above, the nominal value simulation was run over 50 times using SYVAC3-UT2 before the agreement between the two codes became "excellent" (as defined in Section 3.1). Once this level of agreement had been achieved, we began the comparison of the second deterministic simulation, in which all parameters were fixed at their minimum values.

The first comparison of the minimum value simulation revealed that there were still major differences between the two codes. Some of these differences were eventually tracked down (and are documented in the last few comments in item 21 of Appendix A), and SYVAC3-UT2 was modified to correspond to the logic in UTAP2. A repeat of the second deterministic simulation revealed that good agreement had been obtained.

Table 3.2/3 shows the pattern of results obtained. It is apparent that the largest remaining differences all involve water pathways (the variables WATD and FISHD obviously depend on contaminant concentrations in the lake waters; MEATD also depends on these concentrations since caribou and moose are assumed to ingest contaminated water and (for moose) contaminated aqueous plants). Major discrepancies occur at about 500 years (~7%) and at about 1000 years (>8%). The sudden appearance of a difference at 500 years, with its subsequent disappearance at 650 years, suggest that UTAP2 and SYVAC3-UT2 disagreed on the time of depletion of some component of the tailings, such as gypsum (examination of the detailed output from SYVAC3-UT2 shows that gypsum was depleted in layer 2 between 350 and 500 years). It was noted in the previous section that because of discontinuities in the model at depletion times, sudden discrepancies like this one could arise. Attempts to localize the source of the remaining differences were not fruitful, however. Nor was it certain that the differences occurring at two different times were caused by the same difference between the codes. We expect that more detailed output, clustered near 500 and 1000 years, would have allowed us to identify and correct the difference. Alternatively, a more detailed scrutiny and comparison of the codes would also reveal the source of the discrepancy, but this option would take somewhat longer.

After the SYVAC3-UT2 code was modified to correct those discrepancies that were found in this run, the nominal value (first) simulation was rerun. The agreement was still excellent.

Our original intent was to reach excellent or good agreement on each simulation before proceeding to the next. The final results for the minimum value simulation were in good agreement since only six compared values disagreed by more than 2% (but less than 20%). All other values at all other times agreed to within 0.9%. With time running out, we accepted the good agreement and progressed to the third simulation, to determine if the remaining differences would be easier to diagnose there.

Maximum Value Simulation

The third or maximum value simulation was run on SYVAC3-UT2 and compared with the corresponding results from UTAP2. A pattern of differences appeared that was different from the pattern in the minimum value simulation. The cause of the difference was readily identified, and was a case where the SYVAC3-UT2 code did not match its specifications.

After the code was corrected, the results of the maximum value simulation were in excellent agreement; as shown in Table 3.2/4 the differences in all variables at all times are less than 0.4%. The first and second simulations were also rerun, with no significant changes to their results.

The Last Three Randomly-Sampled Simulations

The last three deterministic simulations were also run on SYVAC3-UT2 and compared with the results from UTAP2, but no attempt was made to localize any differences in the two codes. As shown in Tables 3.2/5 to 3.2/7, the results are in excellent agreement; in each of these three simulations, 15 or 16 of the 18 compared values agree to within 2% and all agree to within 20%. Only two variables disagree by more than 2% at some times: they are FISHD and MEATD. Note, however, that dose due to ingestion of water, WATD, has not been compared (these results were not included in the UTAP2 output). If the trends in Table 3.2/3 also apply to Tables 3.2/5 to 3.2/7, then deterministic run 5 (Table 3.2/6) might achieve only good agreement.

Except for the variables FISHD and MEATD, all other values at all times agree to within 0.2% for all three of deterministic simulations 4, 5 and 6.

Summary - Deterministic Comparisons

Tables 3.2/2 to 3.2/7 provide a summary of the (final) results obtained from the deterministic comparisons. Following the criteria documented in Section 3.1, the nominal-value, maximum-value and all three randomly-sampled simulations are in excellent agreement, while the minimum-value simulation is in good agreement. Closer inspection of these tables, in particular Table 3.2/3, shows some trends that suggest some minor differences in SYVAC3-UT2 and UTAP2 may remain.

The second and third deterministic comparisons have demonstrated that the detailed comparison of more than one simulation has merit for probabilistic codes like UTAP2 and SYVAC3-UT2. As noted above, some differences between the two codes were not apparent until the second and third simulations were run. These same differences, or perhaps other differences, are also apparent, to varying degrees, in the last three simulations. The reason is that a different set of input parameters can change the relative importance of different parts of the system model, and thereby highlight errors that were not detectable in a single run of the code.

Time constraints meant that only the first three of the six deterministic simulations could be compared and investigated in detail, and that one of these deterministic simulations did not reach "excellent" status. Nevertheless, we feel that the agreement that was achieved is a strong indication that most of the original differences between UTAP2 and SYVAC3-UT2 have been found. By running six quite different simulations, we have exercised most of the code in SYVAC3-UT2. As a result, it is quite possible that any remaining differences between UTAP2 and SYVAC3-UT2 are of a relatively minor nature.

3.3 Comparison of Probabilistic Results

One of the objectives of this project was the comparison of the results of UTAP2 and SYVAC3-UT2 when both codes were run in their probabilistic mode. In preparation for achieving this objective, a sample two-way analysis of variance (ANOVA) was conducted on two sets of simulations run using a simple model (not a tailings model) in SYVAC3. The objective of the test was to determine if ANOVA could properly identify both insignificant random variations and significant systematic variations. The results were satisfactory and suggested that the criteria based on the ANOVA approach would provide suitable data for a qualitative summary of the probabilistic comparison.

Unfortunately there was no opportunity to apply ANOVA to UTAP2/SYVAC3-UT2 results within the time constraints of the contract. We estimate that another two weeks' effort would have been required to run the probabilistic simulations, extract the appropriate results from the output of both codes, and conduct and interpret the statistical analysis.

In any case, it may be too early to attempt the probabilistic comparison, since the results of the deterministic comparisons are not yet definitive. We feel that, before the probabilistic comparison is attempted, all of the deterministic simulations should be in excellent agreement and the reasons for all differences should be well understood.

4.0 SUMMARY AND RECOMMENDATIONS

Summary

The major objective of this project was to carry out a comparison of UTAP2 and SYVAC-UT2, two probabilistic systems assessment codes that could be used as tools in evaluating the long-term environmental impact of uranium mine tailings. The mine tailings model in SYVAC3-UT2 was derived entirely from documentation of UTAP2, and so the results of the comparison can be used to check that UTAP2 performs the calculations that it was intended to perform. Insofar as the codes agree, the quality assurance of UTAP2 is enhanced, giving its users increased confidence that the code performs as expected.

This objective has been met, to a limited extent. That is, the codes have been compared using six quite different data sets, and a set of differences has been identified between the two codes. The results of the comparison clearly indicate that for the most part UTAP2 is an implementation of the model described in UTAP2 documentation. Every part of the model has been implemented in full, and by and large the equations in the code are those in the model documentation. In short, the scientific description of the model corresponds to the code.

That said, it must be pointed out that in detail there are dozens of ambiguities in the documentation and inconsistencies between the documentation and the code. It is these ambiguities and inconsistencies that account for the 177 detailed comments in Appendix A. Many of these comments address omissions in the documentation. Either an aspect of the model was not clearly explained, or some important fact was missing. For example, initial conditions for many variables were missing. Other comments address minor inconsistencies, such as the use of the constant 8.97 in the code when 8.99 is used in the documentation. Some address more significant differences, such as the undocumented use of complicated terms in a few equations or the absence of some equations. Other comments dwell on the complicated logic in the UTAP2 code. The code uses multiple conditions depending on the depletion of several different chemical species in the tailings, and it is very difficult to completely explain all the alternatives in a narrative document. The net result of all these ambiguities and inconsistencies is that the UTAP2 code itself is still the only completely accurate description of the tailings model.

The comparison was limited in the following ways. First, not all aspects of the model were tested. Some of the aspects not tested include the groundshine dose model, calculations for added lime, calculations for more than two soil layers, time-dependent sampling of net precipitation (NPRCP) and probabilistic sampling. Second, not all the areas of disagreement were resolved. In five of the six simulations compared, excellent agreement was achieved, but in the sixth, only good agreement was reached, and there is evidence in the results of some remaining discrepancies between the two codes. These limitations do not affect the conclusions above.

The second objective of this project, which increased in importance as the work proceeded, was to augment the documentation of the uranium tailings model contained within UTAP2. The written documentation of this model (SENES, 1986) provides a comprehensive description of the scientific basis for the model. However this description is not adequate for the purpose of defining a working computer code. The specifications given in Appendices B and C are the most precise description of the UTAP2 model currently available, short of the code itself. They complement the existing UTAP2 documentation, in that the documentation describes the model in physical and chemical terms, and the specifications describe the model as a data transformation applied to input parameters.

Recommendations

From our experience with this project, we can make a number of recommendations. Some specific recommendations that apply to UTAP2 and this project are:

(1) That all documented differences should be examined carefully to determine whether changes are required in the UTAP2 code or documentation. Item 21 in Appendix A includes 78 comments on the UTAP2 documentation and/or on the UTAP2 code that were made during the test and comparison phases. These have not been discussed with SENES Consultants and should be reviewed by modelling experts. We suspect that in most cases the UTAP2 code is correct, and that comments relate to ambiguous or missing elements of the UTAP2 documentation. (Some of the following points might also resolve these differences.)

(2) That the starting conditions for the uranium tailings system should be given more attention in the documentation. Many problems encountered during the course of this project related to the documentation of the initial conditions, which were too often missing or ambiguous. Often it was not clear when the initial conditions were to be applied. For example, the initial conditions for some variables applied to the starting time t=0, and

others applied to an earlier time t=-DT, where DT was the time step-size.

(3) That the dependence of UTAP2 results on the time step-size (DT) be examined. The time step-size is a parameter introduced into the model as an artifice to avoid having to deal with continuously-varying functions of time. There should be a range of time step-sizes which give equivalent dose values. In these comparisons, however, changing DT from one to ten years changed the dose estimates, and in particular calculated results at t=0 are different. It appears that the dependence on DT is primarily due to its appearance in the initial conditions (although it could also be a convergence problem in the finite difference equations). This characteristic of the uranium tailings model seems to be unrealistic, and should probably be amended.

(4) That the chemical and/or physical discontinuities embedded within the uranium tailings model be investigated further. Discontinuous behaviour of variables in the UTAP2 model made comparisons difficult. One way of resolving this difficulty is to compare detailed results over small time steps on either side of the discontinuities. A better approach might be to re-examine the need for these discontinuities, and to improve the behaviour of the model when they occur.

(5) That the specifications in Appendices B and C be updated whenever the UTAP2 documentation or code is changed. We believe that these detailed specifications contribute substantially to the quality assurance process, but their value will diminish rapidly if they are not kept up to date.

Experience with this project has also shown that comparisons of this type are effective in detecting problems with the documentation and coding of a particular model. To this end, we recommend:

(6) That comparisons of the type documented in this report be repeated whenever extensive revisions are made in subsequent versions of UTAP2.

(7) That methods be sought to streamline the detailed code comparison process. Some possibilities include:

- Specifications: The documentation of a complicated model, such as the uranium tailings model, should include a detailed set of specifications, like those in Appendices B and C. Had they existed prior to the start of this contract, the focus of the effort would have been on the comparison of the two codes, rather than on attempts to produce the detailed model specifications. If they are produced early in the development of a code, they can be very useful in code design. They can also be useful as the basis for a competitive tendering process to develop code for a model.

- Walkthroughs: Our experience has shown that errors do occur at each stage of software development, and that review of software products, such as specifications, is an effective way of finding them. If errors are found early, the cost of fixing them can be substantially reduced. Walkthroughs are a formal set of product reviews in which the developer of a product explicitly shares ownership of the product with a group of reviewers. Newly-prepared specifications should be subjected to walkthroughs, but the walkthrough process must be reorganized (if possible) to improve upon its efficiency. It may be possible to achieve the same benefits by using a fewer number of selected experts for all walkthroughs, by starting the walkthroughs from the top level of specification, and by performing the walkthroughs on all related parts of the specifications (each of which must be fully completed).

- Deterministic comparisons: Deterministic comparisons should be made using running copies of both codes, to facilitate the identification of the sources of differences. The detailed results from UTAP2 were very useful in tracking down differences, but in many cases even more detailed results were needed for quick tracing of discrepancies. Running copies of both codes could be used with a run-time debugger to quickly locate differences by tracing the calculation of all relevant variables.

- Probabilistic comparisons: A set of probabilistic runs can generate large data sets. For example, the probabilistic output from UTAP2 that would have been used in this project consists of tens of thousands of variables to be compared, in files taking up over 6 Mbytes of memory. A common format is needed for probabilistic output files so that data can be readily extracted and compared. Programs to plot or analyze the data would then work on outputs from both codes being compared. Work on such a common format is being carried out by the Probabilistic Systems Assessment Users Group of the OECD/NEA.

- Comparison criteria: The criteria described in Section 3.1 are acceptable for use in these types of comparisons. The criteria used for the comparison of the deterministic simulations were sufficiently precise that the exercise was not trivial. Although this report does not cover a comparison of probabilistic results, we have investigated the criteria based on the ANOVA approach, and we expect that they would be equally acceptable. A definitive criterion is still missing for comparison of distribution tails of dose variables.

(8) That the comparison procedure involve several deterministic simulations as well as a set of probabilistic simulations. Most of the differences detected in this work were found during the comparisons with the first simulation. However other differences were also detected by the second and third simulations, because

each used different sets of input parameters that tended to emphasize different portions of the tailings model. Three deterministic simulations might be insufficient; each additional successful deterministic simulation adds to the confidence in the comparisons without unduly taxing the analytical effort. In addition, more simulations will be required if there are parameters (such as the lime option) that have different discrete values. Once all deterministic simulations have attained excellent agreement (and/or when all differences have an understood cause), a set of probabilistic simulations should be compared.

ACKNOWLEDGEMENTS

The authors are indebted to a number of people who contributed to this work. They include, from WNRE, K.J. Frech, D.B. McConnell, T.W. Melnyk, G.R. Sherman, A.M.M. Skeet and P. Vilks who contributed to the walk-throughs; E.N. Henschell who helped produce the specification figures and A.G. Wikjord who helped polish the draft copy. B.E. Halbert and C. Hallam of SENES Consultants were instrumental in assisting with many difficulties encountered with the documentation of the tailings model, and in preparing the detailed output from UTAP2 for the deterministic comparisons. R.W. Holmes from the NUMP also provided useful comments for the comparison criteria, and for the contents of this report.

REFERENCES

AECB, 1985. Deep Geological Disposal of Nuclear Fuel Waste: Background Information and Regulatory Requirements Regarding the Concept Assessment Phase. Atomic Energy Control Board Regulatory Document R-71.

Andres, T.H., 1985. Features of the SYVAC3 Executive. In Proceedings of the Twentieth Information Meeting of the Nuclear Fuel Waste Management Program. Atomic Energy of Canada Limited Technical Record*, TR-375, Pinawa, Manitoba.

BBS, 1986. PC-OUTLINE, Reference Manual. Brown Bag Software, 2105 South Bascom Avenue, San Jose, CA, 95121.

Dormuth, K.D. and Quick, R.D., 1981. Accounting for Parameter Variability in Risk Assessment for a Canadian Nuclear Fuel Waste Disposal Vault. Int. J. of Energy Systems, 1, pp. 125-127.

Dormuth, K.D. and G.R. Sherman, 1981. SYVAC - A Computer Program for Assessment of Nuclear Fuel Waste Management Systems, Incorporating Parameter Variability. Atomic Energy of Canada Limited Report, AECL-6814, Pinawa, Manitoba.

Goodwin, B.W., 1984. Evolution of SYVAC3. In Proceedings of the Eighteenth Information Meeting of the Nuclear Fuel Waste Management Program. Atomic Energy of Canada Limited Technical Record*, TR-320, Pinawa, Manitoba.

Goodwin, B.W. and E.L.J. Rosinger, 1985. Environmental and Safety Assessment. In Proceedings of the Twentieth Information Meeting of the Nuclear Fuel Waste Management Program. Atomic Energy of Canada Limited Technical Record*, TR-375, Pinawa, Manitoba.

Goodwin, B.W., N.C. Garisto and J.W. Barnard, 1987. An Assessment of the Long-Term Impact of Chemically Toxic Contaminants from the Disposal of Nuclear Fuel Waste. Atomic Energy of Canada Limited Report, AECL-7819 (in preparation).

Goodwin, B.W. and T.H. Andres, 1986. Comparison of the Probabilistic Systems Assessment Codes, UTAP and SYVAC3, Applied to the Long-Term Assessment of Uranium Mill Tailings in Canada. Contract report prepared under contract #0SQ85-00293 for the National Uranium Tailings Program, Canada Centre for Mineral and Energy Technology, Energy, Mines and Resources Canada, 555 Booth Street, Ottawa, Ontario, K1A 0G1.

Goodwin, B.W., T.H. Andres, P.A. Davis, D.M. LeNeveu, T.W. Melnyk, G.R. Sherman and D.M. Wuschke, 1987. Post-Closure Assessment for the Canadian Nuclear Fuel Waste Management Program. Submitted to the International Journal for Radioactive Waste Management and the Nuclear Fuel Cycle.

Guvanasen, V.M., 1985. Preliminary Assessment for the Disposal of Intermediate-Level Reactor Waste. Atomic Energy of Canada Limited Technical Record*, TR-293, Pinawa, Manitoba.

Hamming, R.W., 1971. Introduction to Applied Numerical Analysis. McGraw-Hill, New York.

Harrison, W.C., B.E. Halbert and D.B. Chambers, 1985. Safety Assessment of Uranium Mill Tailings in the National Uranium Tailings Program. Presented at the CNS Conference, Ottawa, May, 1985.

Hoffman, K.J. and G.R. Sherman, 1985. Standards for the Development of Scientific Research Software. Atomic Energy of Canada Limited Technical Record*, TR-291.

Lahey, 1986. Fortran 77 Language System for the Personal Computer (Version 2.11). Lahey Computer System Inc., P.O. Box 6091, Incline Village, Nevada, 89450-6091, 1984.

Murray, M.L., D.B. Chambers, D.I. Beals, B.E. Halbert, T.H. Andres and M. Henrion, 1986. Quality Assurance Documentation on the Uranium Tailings Assessment Program. Draft copy of a report prepared for the Canadian National Uranium Tailings Program, and including material from a report by T.H. Andres entitled "Demonstration of Probabilistic Assessment Procedures Using a Radon Dose Model", dated 1985 June.

Press, W.H., B.P. Flannery, S.A. Teukolsky and W.T. Vetterling, 1986. Numerical Recipes - The Art of Scientific Computing. Cambridge University Press, Cambridge.

PROFORT, 1984. IBM Personal Computer Professional FORTRAN (Version 1.0). Developed by Ryan-McFarland Corporation and distributed by International Business Machines Corporation, P.O. Box 1328-5, Boca Raton, Florida, 33432, 1984.

Rummery, T.R. and Rosinger, E.L.J., 1984. The Canadian Nuclear Fuel Waste Management Program. In Fuel Reprocessing and Waste Management, proceedings of the American Nuclear Society international topical meeting, Jackson, Wyoming, 1984 August 26-29, American Nuclear Society, Lagrange Park, Illinois, pp. 1-14 to 1-32.

SENES, 1985. Probabilistic Model Development for the Assessment of the Long-Term Effects of Uranium Mill Tailings in Canada - Phase II. Volume 1 - Main Report. Volume 2 - Workshop Notes and Topical Discussion Papers. Volume 3 - Probabilistic Analysis User's Manual and Documentation for the Uranium Tailings Assessment Program (UTAP).

SENES, 1986. Probabilistic Model Development for the Assessment of the Long Term Effects of Uranium Mill Tailings in Canada - Phase III. Volume 1 - Main Report. Volume 3 - Uranium Tailings Assessment Program (UTAP) Component Model Documentation. Contract report prepared under contract #OSQ85-00182 for the National Uranium Tailings Program, Canada Centre for Mineral and Energy Technology, Energy, Mines and Resources Canada, 555 Booth Street, Ottawa, Ontario, K1A 0G1.

Sherman, G.R., D.C. Donahue, S.G. King and A. So, 1986. SYVAC2 - A Systems Variability Analysis Code for Assessment of Nuclear Fuel Waste Disposal. Atomic Energy of Canada Limited Technical Record*, TR-317, Pinawa, Manitoba.

Softool, 1984. Programming Environment: Auditor Manual. Softool Corporation, 1984.

Webster, 1985. Webster's New Collegiate Dictionary. Allen & Son Limited, Markham, Ontario.

Wuschke, D.M., A.M. Rice and P.A. Gillespie, 1983. Environmental Assessment of Sub-Seabed Disposal of Nuclear Wastes: A Demonstration Probabilistic Systems Analysis. Atomic Energy of Canada Limited Technical Record*, TR-206, Pinawa, Manitoba.

Wuschke, D.M., P.A. Gillespie, K.K. Mehta, W.F. Heinrich, D.M. LeNeveu, G.R. Sherman, V.M. Guvanasen, D.C. Donahue, B.W. Goodwin, T.H. Andres and R.B. Lyon, 1985. Second Interm Assessment of the Canadian Concept for Nuclear Fuel Waste Disposal. Volume 4: Post-Closure Assessment. Atomic Energy of Canada Limited Report, AECL-8373-4, Pinawa, Manitoba

Wuschke, D.M., K.K. Mehta, K.W. Dormuth, T.H. Andres, G.R. Sherman, E.L.J. Rosinger, B.W. Goodwin, J.A.K. Reid and R.B. Lyon, 1981. Environmental and Safety Assessment Studies for Nuclear Fuel Waste Management. Volume 3: Post-Closure Assessment. Atomic Energy of Canada Limited Technical Record*, TR-127-3, Pinawa, Manitoba.

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* Unrestricted, unpublished report, available from SDDO, Atomic Energy of Canada Research Company, Chalk River, Ontario, K0J 1J0.

APPENDIX A. ANCILLARY DOCUMENTATION FROM SENES

During the specification, design and data preparation phases, some problems and discrepancies were encountered in extracting required information from the material in the SENES report[1]. A number of telephone conversations and letters between SENES and the Whiteshell Nuclear Research Establishment were required to resolve these difficulties.

Since the resultant information forms a significant part of the work described in this report, a full record was kept of the questions passed to SENES and the answers which SENES provided. The following pages are reproductions of letters to and from SENES and of notes taken during telephone conversations with SENES. They are arranged in chronological order, and consist of:

			Page
1.	Letter to B.E. Halbert	1986 Sept 5	A-2
2.	Letter to R.J. Lemire	1986 Sept 11	A-6
3.	Letter to R.J. Lemire	1986 Oct 16	A-8
4.	Letter to B.E. Halbert	1986 Oct 20	A-16
5.	Letter to R.J. Lemire	1986 Nov 4	A-19
6.	Letter to B.E. Halbert	1986 Nov 5	A-27
7.	Letter to B.E. Halbert	1986 Dec 1	A-30
8.	Letter to R.J. Lemire	1986 Dec 2	A-32
9.	Letter to R.J. Lemire	1986 Dec 9	A-37
10.	Letter to R.J. Lemire	1986 Dec 11	A-40
11.	Letter to B.E. Halbert	1986 Dec 22	A-43
12.	Letter to B.E. Halbert	1987 Jan 8	A-45
13.	Letter to R.J. Lemire	1987 Jan 13	A-47
14.	Letter to B.E. Halbert	1987 Jan 21	A-54
15.	Letter to R.J. Lemire	1987 Jan 27	A-57
16.	Letter to B.E. Halbert	1987 Jan 29	A-62
17.	Letter to R.J. Lemire	1987 Feb 3	A-63
18.	Letter to R.J. Lemire	1987 Feb 4	A-69
19.	Notes on a call to SENES	1987 Feb 17	A-71
20.	Letter to B.W. Goodwin	1987 Feb 18	A-72
21.	Notes on remaining questions	1987 Feb-April	A-76

The last item documents some questions that arose during the final preparation of the specifications and/or during the design and coding phases. They were not formally resolved through consultation with SENES due to time constraints. Instead the questions were resolved by the project team at WNRE, and the corresponding assumptions are noted.

1/ SENES, 1986. Probabilistic Model Development for the Assessment of the Long-Term Effects of Uranium Mill Tailings in Canada - Phase III. Volume 3 - Uranium Tailings Assessment Program (UTAP Component Model Documentation. Contract report prepared under contract #0SQ85-00182 for the National Uranium Tailings Program, Canada Centre for Mineral and Energy Technology, Energy Mines and Resources Canada, 555 Booth Street, Ottawa, Ontario, K1A 0S1.

RCB-86-298

1986 September 5

Bruce Halbert
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Dear Bruce;

Further to our conversation of September 3rd, and a follow-up call from Dave Hopper on September 4th, I am enclosing a list of questions that have arisen so far in our work on the NUTP contact. Some questions are probably trivial, and others may have been addressed since the draft report was sent to us. A few questions may require some time.

1. In SENES documents for Phases II and III the distribution for FPRCP is given by Lognormal (123, 18, 84, 156). In a letter SENES to Goodwin (1986-02-13) it is given as Lognormal (123, 0.8, 121, 125), i.e., for a 500 year average. Which should be used?

2. In equation 4.2 the approximation is used that $x_2 \rightarrow \infty$. In Table 4.1 $X_s(t)$=1.0m is given. It appears that the value in Table 4.1 would render invalid the approximation $x_2 \rightarrow \infty$.

3. AEXPT=(1-FVEG)*ATAIL (marked as the tailings area used as the Radon (I assume you mean Radium?) source in Table 3.5 - the program listing). Is this the equation used? It does not seem to appear elsewhere.

4. For consistency, in the air dispersion model, AIRDIS, shouldn't ATAIL be used for the Rn source and AEXPT for the Ra, Pb, U, Th in the calculation of RNGMID?

5. There must be an error in Table 5.2, B=2, as the calculated σ_z for 5000m differs drastically depending on the coefficients used. Also, the meaning of the first column is not clear. I have some idea what stability classes A-->F are, but what does C=4, D=4 etc. mean?

6. Equation 6.8, first term should read $Z_{ij}(t-\Delta t)\exp[-(\beta_{ij} + \lambda_j)t]$?

7. Initial conditions for the soil model are $Z_{ij}=0$ at $t= -\Delta t$?

8. Why is thorium in the SOIL model only ^{232}Th and the uranium ^{238}U when the DUST model uses ^{232}Th + ^{230}Th and natural uranium?

9. Is the distribution for RHOS1 LN(129., 1.3, 20., 450.)? In Table 6.2 it is given as LN(129., 1.3, 20450).

10. It is not clear if FWAT in the SOIL model is the fraction of the total precipitation (after eqn. 6.12) or the net precipitation (section 6.2). Also, why are 4 parameters given for what is described as a triangular distribution. The values are not the same as FNPRCP in GWATER.

11. In Table A.3 should P (NPRCP) be in units of m a^{-1}? Also in the SOURCE the distribution for NPRCP is N(0.4, 0.1, 0.15, 0.65) but in SOIL it is N(0.4, 0.1, 0.1, 0.7). Should these be the same?

12. DEPVEL is given as having units of [m s^{-1}] in Table 6.2 but [m a^{-1}] with respect to equation 6.1?

13. μ_c/ρ_c (E=0.1MeV) from eqn. 7.10 is equal to μ_c/ρ_c (E=0.2 MeV) from eqn. 7.11. What are the correct regression equations?

14. Why is Th ≠ (Th-230 + Th-232) but U = nat-U in GSHINE, and thus differing from the definitions in SOIL and/or DUST?

15. We need
    a) avg. energy for ith radionuclide in jth energy band
    b) energy absorption coefficients for flesh for ith energy band
    c) # of decays for the ith radionuclide in jth energy band
    d) specific activity of ith radionuclide (ENERG, MUFLSH, NNDEC, SPA) not supplied for input to GSHINE. Also, is MUFLSH a constant as stated in the text?

16. Is RHOS the dry soil density or the wet soil density? It appears to be the dry soil density in SOIL but could be a wet soil density in GSHINE. Is DRYRHO in VEGCON equal to RHOS(2)/1000.? I assume SGGWAT in GWATER is the dry density of the sand (and correctly assumed to be different from the soil density in SOIL).

17. In Chapter 6 the definitions of SOILC and SOILCN are not clear. What parameters (in the text) do these correspond to? SOILCN seems to be the parameter used in GSHINE, SOILC seems to be used in VEGCON. (I realize in VEGCON only the soil concentration in the first subsurface layer (layer 2) is needed. Is this SOILC, while the general expression for any soil layer is SOILCN?)

18. Is EMANAT sampled from the same triangular distribution in GSHINE as in RADON?

19. Is GDSE (Table 7.1) simply ΣD^n_T (from eqn. 7.15) and if so, are the units [Sv] as in Table 7.1 or [Sv a^{-1}] as in eqn. 7.14?

20. How does POGWAT (GWATER) differ from TVOID (DUST)? Are the differences deliberate for the saturated and unsaturated zones?

21. Equation 9.19, is $L = \alpha$? If so is the equation correct? In Table 9.5 the deterministic value of α=25 is for X=80.

22. Is ρ_s in Table 9.2 equal to ρ_B in eqn. 9.5?

23. ln(2)/TH(U-238) in Table 9.4 differs slightly from XLAMDA(U-238) in the SOIL model.

24. In eqn. 9.8a is C_{Ra} the same as C(X,t) for Ra-226 at the discharge point (GWATC(i,t))?

25. FNPRCP distribution is LN(0.15, 1.66, 0.07, 0.3) in GWATER, but is LN(0.15, 1.27, 0.07, 0.3) in SOURCE.

26. It would seem the volume of source term discharge from the tailings area to the watershed, SFLOW, might be (NPRCP x ATAIL), although no equation is apparent (at least in Chapter 10). Is this correct?

27. Equations 10.2 and 10.3 include both the concentrations of ions from the body of water upstream of the node of interest plus the concentrations from the tailings source. This appears redundant.

    Should, for example, equation 10.2 be rewritten as:

    $$[Ca]_{n,t} = \frac{Q_{s,t}[Ca]_{s,t} + Q_{n,t}[Ca]_B}{Q_{n,t}} \qquad n=1$$

    $$[Ca]_{n,t} = \frac{Q_{n-1,t}[Ca]_{n-1,t} + (Q_{n,t} - Q_{n-1,t})[Ca]_B}{Q_{n,t}} \qquad n>1 \quad .$$

28. Units for KDPRIM in Table 10.5 should be [m^3 g^{-1}].

From the telephone conversations I understand that you will be forwarding a floppy disk with the STAR data plus a description of the equations used to obtain FWINDT (in DUST), UWIND, FWIND2 (in AIRDIS) etc. I also understand that the revised description of WATEX will incorporate input from the GWATER and erosion models in addition to the water from the watershed and the mixing zone.

Thank you for your help.

Yours sincerely,

ORIGINAL SIGNED BY

Robert Lemire

RL/cr
cc: B. Goodwin ✓

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30259

11 September 1986

Mr. Robert Lemire
Atomic Energy of Canada Limited
Research Company
Whiteshell Nuclear Research Establishment
Pinawa, Manitoba
ROE 1L0

Dear Mr. Lemire:

In response to your questions regarding the Phase 3 input wind data, enclosed is a copy of the AES Star Data files used to create the input wind files.

1. Twenty annual averages
   - the twenty annual average Star Data files were combined into one file, i.e. P1397.F01+P1397.F02+...P1397.F20.

2. One, twenty year average
   - the twenty year average input file was created by averaging the relative frequency distributions by speed class, by direction, by stability class

   - the format of this file was the same as the original Star Data files.

3. Twenty, ten year averages
   - twenty ten year average files were created using the same method which created the twenty year average, i.e. averaged files: (1) P1397.F01 to P1397.F10
     (2) P1397.F02 to P1397.F11
     .
     .
     .
     (20) P1397.F20 to P1397.09.

   - the twenty ten year average files were then combined into one file (as in step 1)

   - the format of this file was the same as the original Star Data files.

...../2

30259
Mr. Robert Lemire
11 September 1986
Page 2

If you have any further questions with regard to the wind input data, please contact me.

Yours very truly,

SENES CONSULTANTS LIMITED

Todd Ellenor

Todd Ellenor
Environmental Engineer

pm

Bruce Received this [illegible]

Robert

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30334

16 October 1986

Mr. Robert Lemire
Atomic Energy of Canada Limited
Whiteshell Nuclear Research Establishment
Pinawa, Manitoba.
ROE 1L0

RE: Response to Questions Regarding the UTAP Phase III Code Documentation

Dear Robert:

Attached please find our response to questions you raised in correspondence to us dated 5 September 1986. We have structured our response to correspond exactly with the numerical order of the questions in your letter. As you will note, we have responded to all but three of the questions you had. I need to discuss these with Doug Chambers (he is out of the office at the present time) and will get back to you shortly on these items.

Several of the points you raised have been corrected in the final version of our documentation. A copy of Volume 3, which is of most interest to you, will be forwarded to you soon. In the meantime, please find enclosed a copy of Volumes 1, 2 and 4 of the Phase III report.

I trust our responses help clarify the points you raised. Please feel free to call to discuss points which you find unclear.

Yours very truly,

SENES CONSULTANTS LIMITED

Bruce E. Halbert

Bruce E. Halbert, M.S.
Principal

ls

Encl.

cc R. Holmes, NUTP

30334
15 October 1986

Response to Questions raised by Mr. Robert Lemire, Whiteshell Nuclear Research Establishment, Atomic Energy of Canada Limited, in correspondence dated 5 September 1986 on the Phase III Probabilistic Assessment Study.

1. Note that the distribution for FPREC (not FPRCP) is specified as being normal not lognormal.

   The distribution N(123, 18, 84, 156) gives the expected annual mean number of days with more than 0.25 mm of precipitation. This distribution is correct if the parameter is sampled annually (sampled each time-step) on any trial. If the parameter is sampled only at the beginning of each trial, then the distribution must be adjusted for the time period of the simulation. The table of values provided to Bruce Goodwin on 13 February 1986, were for a specific run condition and should be used with caution. The values for FPREC in this run were adjusted for a 500 year simulation period, i.e., the standard deviation of the distribution was divided by the square root of the time period, or $18 \div (500)^{0.5} = 0.8$. The minimum and maximum values of the distribution were adjusted accordingly, resulting in the specifications N(123, 0.8, 121, 125).

2. (Response to follow.)

3. The parameter AEXPT, which is calculated in the Erosion Model, is imported to the Dust Source Model where it is used to calculate the amount of dust eroded by wind action from the exposed tailings surface. Due to vegetative growth, the area of the exposed tailings changes with time as indicated in the descriptive writeup for the Erosion Model in Chapter 3. The title on the program listing in Table 3.5 has been changed to alleviate the confusion.

4. The parameter ATAIL is used in the Radon Source Model and the parameter AEXPT is used in the Dust Source Model.

5. Table 5.2 has been revised in the final version of Chapter 5 to clarify the points raised. (See copy of revised Table 5.2 attached.)

6. Correct, the first term of equation (6.8) should read

$$Z_{ij}\,(t-\Delta t)\,\exp\,[-(\beta_{ij} + \lambda_i)t]$$

7. Correct, the initial conditions for the soil model are $Z_{ij} = 0$ at $t = -\Delta t$. We are concerned only with the incremental increase in activity due to the tailings area.

8. (Response to follow.)

9. The correct distribution for RHOS(J) is LN(129, 1.3, 20, 450).

10. The parameter FWAT is the fraction of the net precipitation which moves as surface runoff (i.e. does not infiltrate the soil profile). The distribution of FWAT is given as T(0.02, 0.16, 0.48); the four values referred to in your correspondence must be from a former draft. The parameter FWAT is not the same as FNPRCP. The latter parameter refers to the amount of the net precipitation which penetrates the full depth of the tailings profile and enters the groundwater flow system below the tailings mass. The former parameter relates to the split in the precipitation between that which moves horizontally and that which moves vertically at the top of the soil surface.

11. The parameter NPRCP has units of $m.yr^{-1}$ and a distribution of N(0.4, 0.1, 0.15, 0.65). The values given on Table 6.2 of the Soil Model are incorrect.

12. The parameter DEPVEL has units of $m.s^{-1}$ and the values given in Table 6.2 are in units of $m.s^{-1}$.

13. The correct regression equation for the full range of E values is:

$$\mu_C/\rho_C = 2.7 \times 10^{-3}\ E^{-0.320}$$

Equations (7.10) and (7.11) in the draft documentation have been replaced by the above equation.

14. (Response to follow.)

15. The information requested on number of decays in each energy level, average energy of each energy level, specific activity and attenuation coefficients is provided on the attached Table. The parameter MUFLSH is treated as a constant.

16. The parameter RHOS is the dry bulk density. Identical values are used in both the Soil and Groundshine Models. The parameter DRYRHO is calculated from the expression:

DRYRHO = 1000 x RHOS(2)

to convert the units from $kg.m^{-3}$ to $g.m^{-3}$. Note that this expression is different from that given in your correspondence.

The parameter SGGWAT in the Groundwater Model is the soil density (not bulk density) and is adjusted in the code to take into account porosity.

17. Yes, SOILCN is the general expression for the ith radionuclide in the jth soil layer while SOILC is the soil concentration of the ith radionuclide in soil layer 2.

18. The radon emanation fraction is treated differently in the Radon Source Model (i.e. emanation from tailings) and the Groundshine Model (i.e. emanation from soil). Hence, the parameter is identified as EMANAT in the Radon Source Model with a triangular distribution and as EMFRAC in the Groundshine Model with a constant value.

19. Yes, GDSE is the ΣD_1^n and has units of $Sv.yr^{-1}$.

20. The parameter POGWAT refers to the porosity of the solid medium through which the groundwater flows. For the reference site, the solid medium is considered to be sand with a porosity of U[0.30, 0.36]. The porosity of tailings, identified by the parameter POROS (previously TVOID) in the Dust Model, is different from that of sand and is given a distribution of values of T(0.35, 0.4, 0.45). The differences are not related to the saturated and unsaturated zones of the tailings as suggested in your correspondence but rather to the characteristics of the respective solid materials.

21. Yes, $L = \alpha$. The parameter α should not be present in Table 9.5 since it is a calculated value.

22. No $\rho_S \neq \rho_\beta$
Rather, $\rho_B = (1 - \theta_T)\, \rho_S$

23. The half-life of Th(U-238) = 4.51×10^9yr is correct.
Therefore, $\lambda_u = \ln 2/t_{1/2} = 1.5369 \times 10^{-10}$ or 1.54×10^{-10}. The slight difference in the values in the Groundwater Model and Soil Model writeups is due to round off error.

24. Yes, $C_{Ra} = C(X,t) = GWATC(i,t)$
where X is the distance to the discharge point
and i (in this case) is Ra-226.

25. The parameter FNPRCP has the distribution LN(0.15, 1.27, 0.07, 0.3). The same distribution of values is used in the Groundwater (Subsurface) Transport Model and the Source Model.

26. The source term discharge as surface runoff, SFLOW, is calculated from the relationship:

SFLOW = (NPRCP * ATAIL) - VSR

and VSR = FNPRCP * AVPRCP * ATAIL

where

NPRCP = the net precipitation ($m.yr^{-1}$)

ATAIL = the surface area of the tailings pile (m^2)

FNPRCP = fraction of the precipitation which penetrates the entire tailings depth

AVPRCP = the long term average precipitation ($m.yr^{-1}$)

SFLOW = volumetric flow of the surface discharge from the tailings site ($m^3.yr^{-1}$)

VSR = volumetric flow of tailings porewater moving into the deep saturated zone ($m^3.yr^{-1}$).

27. Equations (10.2) and (10.3) were written in a general form to apply to calculation of calcium and sulphate concentrations at all nodes. The inference is that at $n-1 = 0$, then $Q_{n-1} = 0$ and $C_{n-1} = 0$. Alternatively, the equations can be written in the form proposed in your correspondence.

28. Yes, the units for KDPRIM in Table 10.5 should be $m^3.g^{-1}$.

Table 5.2

POWER LAW EXPONENTS AND COEFFICIENTS FOR σ_Z

Atmospheric Stability Class	Downwind Distance meters $500 < x < 5000$		Downwind Distance meters $5000 < x < 50,000$	
	a	b	a	b
A	0.0002539	2.086	0.0002539	2.0886
B	0.04936	1.1137	0.04936	1.1137
C	0.1014	0.9260	0.1154	0.9109
D	0.2591	0.6869	0.7368	0.5642
E and F	0.2017	0.6020	1.5763	0.3606

Notes:

1) $\sigma_z = a(x+x_0)^b$

2) In this application if σ_z is predicted to be greater than 5000m, σ_z is set equal to 5000m

3) Stability classes E and F are represented by coefficients for class F.

4) Coefficients a and b are from CDM (1973 p. 8).

15. INFORMATION REQUESTED ON ENERGY LEVELS

NUMBER OF DECAYS IN EACH ENERGY LEVEL FOR EACH RADOINUCLIDE

ENERGY LEVEL RADIONUCLIDE	1	2	3	4	5
U	1.18E6	0.0	0.0	1.26E5	0.0
PB	1.45E5	2.795E6	1.58E6	2.27E6	1.52E6
TH	1.2E14	0.0	0.0	0.0	0.0
RA	1.46E12	0.0	0.0	0.0	0.0
RN	1.46E12	2.01E13	1.72E13	6.23E12	6.22E12

AVERAGE ENERGY IN EACH ENERGY LEVEL FOR EACH RADIONUCLIDE(Mev)

	1	2	3	4	5
U	9.7E-2	0.0	0.0	9.10E-1	0.0
TH	5.96E-2	2.63E-1	5.67E-1	9.00E-1	2.57E00
PB	4.7E-2	0.0	0.0	0.0	0.0
RA	1.86E-1	0.0	0.0	0.0	0.0
RN	4.7E-02	3.31E-1	6.09E-1	1.12E0	1.76E0

SPECIFIC ACTIVITY AND ATTENUATION COEF.

U	TH	PB	RA
1.23E7	4.03E6	3.00E15	3.66E13

MU FOR FLESH

ENERGY LEVEL	1	2	3	4	5
	3.0E-3	3.0E-3	3.0E-3	3.0E-3	3.0E-3

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of Canada Limited
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RCB-86-364

October 20, 1986

Bruce Halbert
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Dear Bruce;

Thank you for your response to the questions I raised (received October 18th), and also for the floppy disk with the STAR data. The disk is readable on our equipment. We also asked for the equations used to obtain FWINDT (in DUST), UWIND, FWIND2 (in AIRDIS) etc. These have not been received. The calculations required are perhaps obvious, but we must be certain that our analysis is identical to yours.

I am enclosing another batch of questions that have arisen since I last wrote. From our conversation of October 16th I understand that an updated version of the Phase III documents will be mailed to me during the week of October 20th.

29. Why is DUNSAT sampled from Constant (1.0) in RADON, but from Uniform (0.75, 1.25) in TSOURC ?

30. $K^\circ_s(BaSO_4)$ is given as 1.07×10^{-4} $mol^2\ m^{-6}$ on page 3-76 of SENES Vol. 3, but as a constant equal to 5.04×10^{-4} $mol^2\ m^{-6}$ on page 11 of Table A.3. Which is correct?

31. $K_f(BaSO_4)$ is given a nominal value of 5.01×10^{-1} $m^3\ mol^{-1}$ but a distribution of "Constant (5.01×10^{-4} $m^3\ mol^{-1}$)" in Table A.3, pg. 11. Which is correct? The former value is in agreement with the one given on page 3-76 of SENES Vol. 3, and is probably correct.

32. A background value of 0.1 [$mol\ m^{-3}$] is included in the calculation of VCONC(6,2,3) (equation 3.3.14) in the TSOURC modules. This is not consistent with the 0.071 [$mol\ m^{-3}$] selected for VTSO4B in WATEX. The values for the calcium concentrations also do not agree.

33. Equation 3.3.15b as derived from equation 3.3.14 contains a term to include the background sulphate concentration from precipitation. Equations 3.3.22 and 3.3.36 have been written neglecting this extra term. Should it have been included?

34. Should "k" in equations 3.3.50 and 3.3.51 be k′ ? Also, in equation 3.3.51 "t" should be Δt. Should the precipitation term also be included in equation 3.3.51 as in equation 3.3.15b (see item 34) ?

35. $K^\circ_{s,BaSO_4}$ has a value of 5.04×10^{-4} in Table A.3 and 5×10^{-4} in Table 3.4.

36. $K_{f,PbSO_4}$ has a value of 5.0×10^{-1} in Table A.3 and 5.01×10^{-1} in Table 3.4.

37. In the DUST module it is stated that $C_i = C_i(t)$ = surficial concentration of the ith radionuclide at time t (pg. 4-7). Table 4.2 defines C_i in the same way, but lists the "Computer Symbol" as CONC(i,1,2) i=1,4. According to Appendix A, Table A.2, CONC(i,1,2) would be the solid phase concentration at "previous time step (t-Δt)". Table 4.1 uses radium concentration CONC(4,i,3) i=1,2 – i.e., concentrations for time t. Which time should be used for these source terms?

38. In Table A.3, pg. 10 should $[Ra_s]^0_1$ be CONC(4,1,1) rather than CONC(4,1,3)? CONC(4,1,3) is $[Ra_s]_1$ (pg. 15 of Table A.3). Is there a similar problem with CONC(4,i,3) i=2,3,4 on page 10? Is $[U_L]^\circ_{\lambda_w}$ = CONC(1,2,1) in Table A.3, pg. 6? I believe this problem also occurs with several other terms in the Table.

39. Am I correct to assume that in equation 3.3.68 the value for pH should be that calculated from equation 3.3.53 rather than 3.3.54 because the solution at the layer boundary (at distance h_t) will always be in contact with both the calcite and gypsum until the unsaturated layer is completely depleted in gypsum ?

40. There is an error in equation 3.3.68. The entire expression should be divided by g_o, not just the first term.

41. $[U_s]_t$ and $[U_s]_{t-\Delta t}$ have units $[Bq\ m^{-3}]$ on page 12 of Table A.3 but $[mol\ m^{-3}]$ on page 3-67.

42. Is $[SO_4^{2-}]_{T,1}$ in equation 3.6.17 equal to WCONC(7,1,3)/1000.

43. I don't seem to have made myself clear concerning the use of ATAIL and AEXPT in the Air Dispersion Model, Chapter 5 of Vol. 3 (my previous question 4). Equation 5.4 requires a value for the tailings area A_o, and Table 5.1 indicates ATAIL has been used. For consistency, shouldn't ATAIL be used for the Rn source and AEXPT for the Ra, Pb, U, Th in the calculation of RNGMID ?.

44. Is FWAT the fraction of the net precipitation "that leaches into soil" (pg. 6-5, Vol. 3) or the fraction that "does not infiltrate the soil profile" (your letter of October 15, 1986, answer to my question 10).

45. In you letter of October 15, 1986 the values supplied for Th and Pb (in the Table of information re my question 15) appear to be transposed in the table giving the number of decays in each level for each radionuclide (NNDEC)

46. Your letter (October 15, 1986, answer to question 18)says EMFRAC ≠ EMANAT, but no value has been given for EMFRAC.

47. In your letter of October 15 (answer to my question 22) you state that $\rho_B = (1-\Theta_T) \times \rho_s$, but I cannot find this equation in Vol. 3, nor a value or equation for Θ)

Yours sincerely,

Robert Lemire

Robert Lemire

cc B. Goodwin

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30334

4 November 1986

Mr. Robert Lemire
Atomic Energy of Canada Limited
Whiteshell Nuclear Research Establishment
Pinawa, Manitoba.
ROE 1L0

RE: Response to Questions Regarding the UTAP Phase III Code Documentation

Dear Robert:

Attached please find our response to questions you raised in correspondence to us dated 20 October 1986. We have structured our response to correspond exactly with the numerical order of the questions in your letter.

I trust our responses help clarify the points you raised. Please feel free to call to discuss points which you find unclear.

Yours very truly,

SENES CONSULTANTS LIMITED

Bruce E. Halbert

Bruce E. Halbert, M.S.
Principal

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Attach.

cc R. Holmes, NUTP

30334
4 November 1986

Response to Questions raised by Mr. Robert Lemire, Whiteshell Nuclear Research Establishment, Atomic Energy of Canada Limited, in correspondence dated 20 October 1986 on the Phase III Probabilistic Assessment Study.

29. The parameter DUNSAT is sampled from a uniform distributions with the attributes (0.75, 1.25). The parameter is sampled only once on any particular trial and the same value is used in both the RADON and SOURCE (identified as TSOURC in your letter) models.

30. The correct value for the parameter KSBAR ($K^o_{s,BaSO4}$) is 1.07×10^{-4} $mol^2.m^{-6}$.

31. The correct value for the parameter KFBAR ($K_{f,BaSO4}$) is 5.01×10^{-1} $m^3.mol^{-1}$.

32. The calcium and sulphate values input as background levels in the source model (SOURCE) were selected to characterize precipitation. The calcium and sulphate values input as background levels in the watershed model (WATEX) on the other hand, were selected to characterize the quality of runoff water from the watershed. Since precipitation quality will be altered on contact with vegetation and soil, it is reasonable that the runoff quality will differ from the precipitation quality.

33. The background sulphate concentration of 0.1 $mol.m^{-3}$ was left out of equation (3.3.22) on purpose to simplify the calculations. The logic was that the precipitation contribution to the sulphate concentration is insignificant relative to the contribution from pyrite oxidation over the time period for which the equation applies (i.e. until gypsum depletion occurs between 100 and 200 years).

The background sulphate concentration is included in the final version of equation (3.3.36).

34. In the final version of the report, k is indeed noted to be k' in equations (3.3.50) and (3.3.51). You are quite correct to state that the term t should be Δt in equation (3.3.51). The background sulphate concentration of 0.1 $mol.m^{-3}$ has been included in the final form of equation (3.3.51).

35. As previously noted the correct value for the parameter KSBAR ($K^o_{s,BaSO4}$) is 1.07×10^{-4} $mol.^2.m^{-6}$. The values given on Tables 3.4 and A.3 are incorrect.

36. The correct values for the parameter KFLEAD ($K_{f,PbSO4}$) is 5.01×10^{-1} $m^3.mol^{-1}$. The difference between the values given in Tables 3.4 and A.3 merely reflects round off.

37. The correct computer symbol for the parameter C_i is:

$$C_i = C_i(t) = \text{CONC }(i,1,3)$$

38. Your question regarding the designation of initial conditions as code 1 or code 3 is an interesting one. It is true that the initial solid phase concentration of Ra-226 in the upper tailings layer, $[Ra_s]^o_1$, should be designated as CONC (4,1,1). Indeed within the initiation subroutine in the SOURCE model it is designated as such. However, for use in all subsequent calculations in the SOURCE model it must be designated as CONC (4,1,3), that is it is now the Ra-226 concentration for the current time when t=0 years. Thus, once CONC (4,1,1) has been computed in the initiation subroutine, the last step involves setting CONC (4,1,3) = CONC (4,1,1). Both values are saved but only CONC (4,1,3) is carried forward and used as input in the other subroutines in SOURCE. The same argument holds for the other parameters in Table A.3. For this reason we have chosen to designate the initial values for all relevant parameters given

in Table A.3 by the current time code (3) rather than the initial time code (1).

39. Yes, you are correct to assume that the pH in equation (3.3.68) (equation (3.3.65) in the final report) should be calculated using equation (3.3.53) (equation (3.6.25) in the final report).

40. Equation (3.3.68) (equation (3.3.65) in the final report) is correct in the final report. One of the brackets was indeed missplaced in the draft report you are referring to.

41. Uranium and thorium are calculated on a mass basis throughout and converted to an activity basis as the last step in the calculation sequence. Hence the units given for uranium in equations (3.8.4) and (3.8.5) are correctly expressed on a mass basis as $mol.m^{-3}$. Similarly, the units given in Table A.3 for $[U_S]_t$ or $[U_S]_{t-\Delta t}$ are correctly expressed on an activity basis ($Bq.m^{-3}$).

42. Yes, $[SO_4]_{\Gamma,1}$ = WCONC(7,1,3)/1000 in equation (3.6.17).

43. No. The value of A_0 in equation (5.4) remains the same in either calculation. The diameter of the tailings area does not change due to vegetation growth. Rather the effect of vegetation is to reduce the effective tailings surface area which contributes to wind erosion losses and thus to the effective Ra, Pb, U and Th loading carried with the wind blown dust. Vegetation is not known to reduce the radon flux hence the whole tailings surface (ATAIL) is considered to act as the radon source.

44. The description in the final version of Chapter 6 of Volume 3 I hope clarifies your question regarding the parameter FWAT. It is the fraction which "does not infiltrate the soil profile."

45. You are indeed correct. The listing given on number of decays in each energy level for thorium and lead are transposed. A correct listing is

attached as Table 1. The data entry in UTAP is correct. The error on the table was made when the data extracted from the code was reorganized and labelled to make it more readible.

46. The parameter EMFRAC is given a constant value of 0.2 on Table 7.1 of the final report. In contrast, the parameter EMANAT is specified as being trianguarly distributed with the following range of values (0.02, 0.2, 0.9).

47. The equation relating bulk soil density (ρ_b) to soil density (ρ_s) is not given in Volume 3. It is imbedded in the code. We have confused the issue however, by introducing the parameter θ_T rather than the parameter n (porosity). Values for the parameter n are given on Table 9.2 in the final report. To reiterate, the equation is:

$$\rho_b = (1 - n)\rho_s$$

General: Wind Data Averaging Calculations

The formula used in the UTAP code for calcuting FWIND2, UWIND, FWIND1(d) and FWINDT from the STAR data are given below. A sample printout of the AES format for the wind data is attached as Table 2.

$$\text{FWIND2 } (d,s) = \sum_{v=1}^{6} \text{FWIND } (d,s,v,n)$$

$$\begin{aligned}\text{UWIND } (d,s) = [&1.50 \times \text{FWIND } (d,s,1,n) + \\ &2.46 \times \text{FWIND } (d,s,2,n) + \\ &4.47 \times \text{FWIND } (d,s,3,n) + \\ &6.93 \times \text{FWIND } (d,s,4,n) + \\ &9.61 \times \text{FWIND } (d,s,5,n) + \\ &12.52 \times \text{FWIND } (d,s,6,n)] / \sum_{v=1}^{6} \text{FWIND } (d,s,v,n)\end{aligned}$$

$$FWIND1\ (d) = \sum_{s=1}^{6} \sum_{v=4}^{6} FWIND\ (d,s,v,n)$$

$$FWINDT = \sum_{d=1}^{16} \sum_{s=1}^{6} \sum_{v=4}^{6} FWIND\ (d,s,v,n)$$

where

d = direction 1→16

s = stability class 1→6

v = velocity class 1→6

n = sample year

TABLE 1

15. INFORMATION REQUESTED ON ENERGY LEVEL

NUMBER OF DECAYS IN EACH ENERGY LEVEL FOR EACH RADOINUCLIDE

ENERGY LEVEL RADIONUCLIDE	1	2	3	4	5
U	1.18E6	0.0	0.0	1.26E5	0.0
TH	1.45E5	2.795E6	1.58E6	2.27E6	1.52E6
PB	1.2E14	0.0	0.0	0.0	0.0
RA	1.46E12	0.0	0.0	0.0	0.0
RN	1.46E12	2.01E13	1.72E13	6.23E12	6.22E12

AVERAGE ENERGY IN EACH ENERGY LEVEL FOR EACH RADIONUCLIDE(Mev)

	1	2	3	4	5
U	9.7E-2	0.0	0.0	9.10E-1	0.0
TH	5.96E-2	2.63E-1	5.67E-1	9.00E-1	2.57E00
PB	4.7E-2	0.0	0.0	0.0	0.0
RA	1.86E-1	0.0	0.0	0.0	0.0
RN	4.7E-02	3.31E-1	6.09E-1	1.12E0	1.76E0

SPECIFIC ACTIVITY AND ATTENUATION COEF.

U	TH	PB	RA
1.23E7	4.03E6	3.00E15	3.66E13

MU FOR FLESH

ENERGY LEVEL	1	2	3	4	5
	3.0E-3	3.0E-3	3.0E-3	3.0E-3	3.0E-3

SAMPLE PRINTOUT OF AES FORMAT FOR WIND DATA.

V=1,6

0-3 | 4-6 | 7-10 | 11-16 | 17-21 | 21+

d=1-16

S=1-6

FWIND(d,S,V,n)

```
0.000410.000280.000000.000000.000000.00000
0.000380.000120.000000.000000.000000.00000
0.000300.000150.000000.000000.000000.00000
0.000100.000060.000000.000000.000000.00000
0.000050.000020.000000.000000.000000.00000
0.000010.000010.000000.000000.000000.00000
0.000030.000030.000000.000000.000000.00000
0.000040.000030.000000.000000.000000.00000
0.000190.000150.000000.000000.000000.00000
0.000290.000170.000000.000000.000000.00000
0.000290.000190.000000.000000.000000.00000
0.000250.000200.000000.000000.000000.00000
0.000490.000260.000000.000000.000000.00000
0.000260.000180.000000.000000.000000.00000
0.000120.000080.000000.000000.000000.00000
0.000210.000100.000000.000000.000000.00000
0.002110.001650.000930.000000.000000.00000
0.001920.001570.000750.000000.000000.00000
0.001420.000770.000540.000000.000000.00000
0.000700.000280.000150.000000.000000.00000
0.000830.000230.000150.000000.000000.00000
0.000410.000100.000050.000000.000000.00000
0.000430.000120.000070.000000.000000.00000
0.000610.000350.000240.000000.000000.00000
0.001380.001270.001320.000000.000000.00000
0.001320.001310.000980.000000.000000.00000
0.001550.001520.001220.000000.000000.00000
0.001380.001520.000880.000000.000000.00000
0.002270.001800.001350.000000.000000.00000
0.001160.001010.000740.000000.000000.00000
0.001070.000800.000520.000000.000000.00000
0.001040.000760.000310.000000.000000.00000
0.000980.002000.003640.000350.000020.00001
0.001170.002030.002700.000110.000000.00000
0.001100.001570.002160.000180.000010.00000
0.000640.000690.000990.000090.000000.00000
0.000700.000790.001450.000150.000010.00000
0.000670.000460.000700.000050.000000.00000
0.000670.000520.000660.000070.000000.00000
0.000700.000830.001790.000330.000030.00001
0.001150.001680.007320.001960.000150.00004
0.000740.001340.004530.000940.000030.00000
0.000670.001290.004820.001030.000020.00000
0.000710.001280.003210.000510.000050.00002
0.001110.002000.006260.001430.000210.00002
0.000810.001330.004520.001110.000200.00003
0.000770.001110.003090.000600.000100.00002
0.000650.000910.002090.000200.000020.00001
0.002440.003680.009810.015030.002830.00043
0.002510.003980.008840.010610.002150.00043
0.002190.003630.009480.013360.003420.00099
0.002290.003550.009970.012710.003830.00097
0.003560.005030.013370.013500.003680.00090
0.002610.003540.008110.007960.002180.00047
0.002470.003380.007630.005870.001310.00016
0.002560.004090.011150.011480.002650.00056
0.003770.005830.017
```

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RCB-86-387

November 5, 1986

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Dear Bruce;

Thank you for sending the final version of the report to NUTP. A number of problems I have had are cleared up in the new Volume 3. However, as I have progressed through the equations of the SOURCE model a few more questions have arisen as noted below.

48. In equation 3.10.23 the first exponential term should probably read $(-\lambda_{Ra-226}\ \Delta t)$ not $(\lambda_{Ra-226}\ \Delta t)$.

49. $[Ra_s]_1$ (CONC(4,1,3)) has units of $[\mathrm{mol\ m^{-3}}]$ on page 3-86 but $[\mathrm{Bq\ m^{-3}}]$ in Table A.3 (pg. 15). Similarly the units for $[Pb\text{-}210_s]_1$ differ on pg. 3-94 and in Table A.3.

50. In equation 3.11.7 there should be parentheses around the last two exponential terms.

51. Should equation (3.5.2) read $[SO_4^{2-}]_{p,mix,t}$ instead of $[SO_4^{2-}]_{p,mix,t-\Delta t}$ (twice)? Similarly for equation (3.5.5) with respect to $[Fe^{2+}]_{mix,t-\Delta t}$?

52. The ingrowth terms described in the "SURFACE WATER DISPERSION MODEL are not consistent with those used in the SOURCE module, and are probably incorrect:

$$\lambda_{Ra}/(\lambda_{Ra} - \lambda_{Th}) \quad \text{instead of} \quad \lambda_{Th}/(\lambda_{Ra} - \lambda_{Th})$$

53. The dimensions vary for the terms in equation 3.10.35. There are two different parameters here, both referred to as $[Ra]_{in}$. The term on the LHS of equation 3.10.35 corresponds to SUMBAR in Table A.3, however it should have units of $[\mathrm{mol\ m^{-2}}]$ for comparison with M_{Ra}° in equation 3.10.36. The summation is not really over $[Ra]_{in}$, but of terms like that on the RHS of equation 3.10.35. The same problem applies for the corresponding terms for lead (3.11.17).

54. In equations 3.10.20, 3.10.27, 3.11.3 should the concentrations $[Th_L]\lambda_w{}^{Th}$, $[Th_L]_{mix}$ and $[Ra_L]\lambda_w$ correspond to the concentrations at $t-\Delta t$ or at t ?

55. At equation 3.11.9 I believe h_{Ra} should read h_{Ba}.

56. $M_{Pb}{}^{\circ}$ is not defined in section 3.7.4, although so noted on page 3-97. I assume it is given by:

$$M_{Pb}{}^{\circ} = [Pb\text{-}210_s]^{\circ} \times (\lambda_w + \lambda_{mix}).$$

57. The text of section 3.11 contains several cryptic comments, most of which are probably typo's. For example, above equation (3.11.14) is the line

"unsaturated zone contains $PbSO_4$ (i.e. $h_pb<\lambda_w$)",

however, the second condition two lines below reads

"unsaturated zone depleted of $BaSO_4$ (i.e. $h_{Pb}\geq\lambda_w$)" .

Which is correct ? The first seems more reasonable. Again, above equation (3.11.20) is another reference to $BaSO_4$. Should this read $PbSO_4$, and should the fourth line of page 3-98 read $\underline{Pb}SO_4$?

58. I am confused about how the radionuclides from the erosion of the tailings pile are incorporated in the surface water dispersion models. In Chapter 3 of Vol 3, page 3-130 it is stated:

> " The total sediment leaving the tailings pile has been assumed to be instantaneously deposited in the first segment of the river/lake system at the bottom of the next time increment. A fraction of the activity in the sediment is assumed to instantly dissolve in the river/lake segment. The balance of the activity remains bonded to the sediment, settles, and becomes part of the bottom sediments of the lake/river."

From this I expected the input to the watershed from erosion to be some quantity of solid (T_m) with radionuclide concentrations CONC(i,1,3), i=1,2,3,4. (Is RHOTAL the appropriate density for the conversion of T_m to a volume of solid ?) I also expected to see some parameter representing the fraction of material assumed to dissolve (perhaps a different parameter for each radionuclide).

In Chapter 10 I find that what is required is a "sediment flux" in units of ($g\ m^{-2}\ a^{-1}$) for which I can find no equation (I assume this is the mass of solids (kg) divided by the area of the lake at node 2 (m^2), divided by the time interval Δt ?). I see nothing to indicate there is a fraction dissolved, although as the radionuclides in layer 1 of the tailings have non-zero concentations (WCONC(i,1,3)), some dissolution must occur. How was this accounted for ?

59. In section 8.4 a value is required for an average air concentration of the radionuclides over the watershed (from section 5.1). Section 5.1 is very sketchy about how the watershed average was calculated. You sent the STAR data, and from chapter 10 we know which watershed nodes are in which sectors, but I cannot find anything that tells what fraction of the watershed (for each node or overall) is in each sector. It is obvious, for example, from Figure 10.1, that the watershed for the lake between nodes 6 and 7 encompasses sections of sectors 8, 9 and 10, with portions both inside and outside ring 4. Therefore, this portion of the watershed area needs to be divided into six subareas for the purposes of calculating radionuclide concentrations resulting from the deposition of airborne material. Could you please supply the relevant data.

60. Table 3.6 lists the parameters BSOIL, CSL and PEROM as "SPECIFIED IN CODE". Could you please supply the data ? It would appear that the value taken for PEROM is always zero (bottom of pg. 3-120) and that the value for BSOIL is always 2 (top of pg. 3-121). Could you please confirm if this is so ?

61. In the SOIL model it is necessary to convert the value for DEPVEL from [m s^{-1}] to [m a^{-1}]. In working with the Phase II study Bruce Goodwin found it was necessary in checking output that we use exactly the same value you have for such conversions. What number have you used in your computer programme for the number of seconds in a year ?

62. In Table 8.5 you refer to SPTCB(i), i=1,4. Should this be SPTCL(i) or ?

Yours sincerely,

Robert Lemire

cc B. Goodwin ✓

RCB-86-410

December 1, 1986

Bruce Halbert
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Dear Bruce;

A few more questions have arisen (as noted below) in addition to those in my letter of November 5th. Primarily these questions are being asked in order that we can document places where there are ambiguities. The first three questions are old ones (from September) to which I have received no answer. I assume they got mislaid.

2. In equation 4.2 the approximation is used that $x_2 \rightarrow \infty$. In Table 4.1 $X_s(t)$=1.0m is given. It appears that the value in Table 4.1 would render invalid the approximation $x_2 \rightarrow \infty$.

8. Why is thorium in the SOIL model only ^{232}Th and the uranium ^{238}U when the DUST model uses ^{232}Th + ^{230}Th and natural uranium?

14. Why is Th ≠ (Th-230 + Th-232) but U = nat-U in GSHINE, and thus differing from the definitions in SOIL and/or DUST?

63. The equation defining the depth of the bottom layer is different below equations 3.7.10 and 3.8.5. The latter equation is almost certainly the correct form.

64. Is the depletion of the lime required to be complete at t or at t-Δt in order that KRATE and SFLUX will revert to the values they would have in the scenario with no added limestone ?

65. In equation 3.3.69, I believe the factor of 1000 should be multiplied by the entire expession, not just the first term.

66. There are trivial differences in the exponents on one of the terms in equations 3.3.65 ($10^{2pH-16.46}$) and 3.3.68 ($10^{2pH-16.47}$) and elsewhere. Which is correct ?

67. In equation 3.3.5 the bold RH bracket should precede "exp".

68. In equation 3.6.23 the pH of the lower unsaturated zone is dependent on the calcium and sulphate concentrations at the bottom of the unsaturated zone. These concentrations require the value of the ratio (d ≡ DELT) between free sulphate and total sulphate (equations 3.3.39 and 3.3.40). In turn the value of DELT depends on the pH. Am I correct to assume these calculations are done iteratively to self-consistency at each time step ? If so, the order of the iteration between these variables should not matter. If, however, one of the values relies directly on another from a previous time interval (for example, if pH(t-Δt) is used in equation 3.3.38 without further iteration after pH is calculated from equation 3.6.23) then we must know the order of the calculations in your program.

Yours sincerely,

ORIGINAL SIGNED BY

Robert Lemire

cc B. Goodwin ✓
R.W. Holmes

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2 December 1986

Mr. Robert Lemire
Atomic Energy of Canada Limited
Whiteshell Nuclear Research Establishment
Pinawa, Manitoba.
ROE 1L0

RE: Response to Questions Regarding the UTAP Phase III Code Documentation

Dear Robert:

Attached please find our response to questions you raised in correspondence to us dated 5 November 1986. We have structured our response to correspond exactly with the numerical order of the questions in your letter.

I trust our answers help clarify the questions you raised. Please feel free to call to discuss points which you find unclear.

Yours very truly,

SENES CONSULTANTS LIMITED

Bruce E. Halbert

Bruce E. Halbert, M.S.
Principal

ls

Attach.

cc R. Holmes, NUTP

Specialists in Energy, Nuclear and Environmental Sciences

RESPONSE TO QUESTIONS raised by Mr. Robert Lemire, Whiteshall Nuclear Research Establishment, Atomic Energy of Canada Limited, in correspondence dated 5 November 1986 on the Phase III Probabilistic Assessment Study.

48 You are correct, the first term in equation (3.10.23) should read $\exp(-\lambda_{Ra-226}\,\Delta t)$.

49 In the UTAP code, the solid and liquid phase concentrations of all chemical and radiological species are calculated on mass basis. As a final step in the calculation sequence, the radionuclide concentrations are converted to an activity basis (i.e. as $Bq.m^{-3}$). Hence, the units reported in Table A.3 for CONC (i,j,k) and WCONC (i,j,k) for the radionuclides are specified as $Bq.m^{-3}$. As previously noted however, the radionuclide inventories are calculated on a mass basis and the discussion in Chapter 3 of Volume 3 develops the appropriate equations for estimating the radionuclide concentrations on a $mol.m^{-3}$ basis. Hence the units given for the terms in the equations are correct.

50. Yes, there should be brackets around the last two exponential terms in equation (3.11.7).

51. No. We have chosen to calculate the change in $[SO_4^{2-}]$ and $[Fe^{2+}]$ concentrations in layer 4 during the current time step as a function of what was in the above layer during the previous time step. Our rationale is that the quality of the porewater moving from the mixing zone (layer 3) to the deep saturated zone (layer 4) during a time step will most closely reflect the quality than existed in the mixing zone at the start of the timestep (i.e. $t-\Delta t$). We are making an allowance therefore for the large dilution capacity of the water stored in the mixing zone and the assumption that only a small fraction is displaced downward during any timestep Δt.

52. The ingrowth terms described in the Surface Water Dispersion Model are indeed incorrect as described. For the ingrowth of Pb-210 from Ra-226

the equations on the top of page 10-30 should read:

$$\ldots\ldots\frac{\lambda_{Ra-226}}{\lambda_{Pb-210}-\lambda_{Ra-226}}\ldots\ldots\text{instead of }\ldots\ldots\frac{\lambda_{Pb-210}}{\lambda_{Pb-210}-\lambda_{Ra-226}}$$

Similary for the ingrowth of Ra-226 from Th-230 the equations on the bottom of page 10-30 should read:

$$\ldots\ldots\frac{\lambda_{Th-230}}{\lambda_{Ra-226}-\lambda_{Th-230}}\ldots\ldots\text{instead of }\ldots\ldots\frac{\lambda_{Ra-226}}{\lambda_{Ra-226}-\lambda_{Th-230}}$$

53. You are correct to note that there are really two different parameters in equation (3.10.35) and also in equation (3.11.17). The summation sign was meant to convey the difference between $[Ra]_{in}$ and $\Sigma[Ra]_{in}$ in equation (3.10.35) and between $[Pb]_{in}$ and $\Sigma[Pb]_{in}$ in equation (3.11.17). As noted, the units for $[Ra]_{in}$ and $[Pb]_{in}$ are $mol.m^{-3}$ while the units for $\Sigma[Ra]_{in}$ and $\Sigma[Pb]_{in}$ are $mol.m^{-2}$.

54. The concentrations for $[Th]_{\lambda w}$, $[Th]_{mix}$ and $[Ra_L]_{\lambda w}$ in equations (3.10.20), (3.10.27) and (3.11.3) respectively, are all for time t.

55. Yes, h_{Ra} in equation (3.11.9) should read h_{Ba}.

56. The parameter M^o_{Pb} is computed from:

$$M^o_{Pb} = X^o_{Pb-210/PbSO4} \quad [PbSO_4]^o \, (\lambda_w + \lambda_{mix})$$

where:

M^o_{Pb} = total Pb-210 initially associated with $PbSO_4$ in the unsaturated and mixing zones ($mol.m^{-2}$)

$X^o_{Pb-210/PbSO4}$ = initial mole fraction of Pb-210 in $PbSO_4$

$[PbSO_4]^o$ = initial concentration of $PbSO_4$ in the tailings ($mol.m^{-3}$)

λ_w = depth of the unsaturated zone (m)

λ_{mix} = depth of the mixing zone (m)

57. The lines above and below equation (3.11.14) should read:

"a) unsaturated zone contains $PbSO_4$ (i.e. $h_{Pb} < \lambda_w$)"

"b) unsaturated zone depleted of $PbSO_4$ (i.e. $h_{Pb} \geq \lambda_w$)"

Similarly, the line below equation (3.11.15) should read:

"In case 1(b), $PbSO_4$ is ...."

The line at the top of page 3-98 should read:

"The value for $[Pb]_{in,4}$ depends on $PbSO_4$...."

Also, the line below equation (3.11.20) should read:

"Case 2: mixing zone depleted of $PbSO_4$"

58. The radionuclides carried with the eroded solids from the tailings area are added directly to node 1 on the watershed. The total mass activity of each radionuclides carried with the solids is assumed to dissolve completely at node 1 and is subsequently redistributed to the solids in the first downstream lake (node 2) by the application of distribution coefficients specific to each radionuclide. The calculation sequence thus involves the following steps:

1. calculate mass activity of radionuclide i at node 1 = [mass activity input from tailings area surface runoff] + [mass activity input from groundwater discharge] + [mass activity input from eroded tailings]

2. calculate solids surface loading on lake at node 2 = [eroded solids mass from tailings/lake area] + [sediment flux from Table 10.2]

3. calculate the radionuclide inventories in the lake water column and lake sediment via equations (10.29) and (10.30) and the radionuclide concentrations in the lake water column and sediments by equation (10.32) and equation (10.33) respectively.

The appropriate density of the tailings solids is given by the parameter RHOTAL. The sediment flux referenced in Chapter 10 is a specified input parameter (see Table 10.2).

59. (Response to follow)

60. The values for the parameters identified on Table 3.6 as "specified in code" are given the following values:

BSOIL - 2.0
CSL - 5.0
PEROM - 0.0

61. Yes, the value of DEPVEL must be converted from $m.s^{-1}$. The multiplier used is:

$$86400\ s.d^{-1} \times 365\ d.a^{-1} = 3.1536 \times 10^{7}\ s.a^{-1}$$

62. Yes, the parameter denoted as SPTCB(i) in Table 8.5 should read SPTCL(i).

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9 December 1986

Mr. Robert Lemire
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Whiteshell Nuclear Research Establishment
Pinawa, Manitoba
ROE 1L0

Re: Response to Questions Regarding the UTAP Phase III Code Documentation

Dear Robert:

Attached please find our response to questions you raised in correspondence to us dated 1 December 1986. We have structured our response to correspond exactly with the numerical order of the questions in your letter.

I trust our answers help clarify the questions you raised. I will forward shortly our response to residual questions from previous inquiries. Please feel free to call to discuss points which you find unclear.

Yours very truly,

SENES CONSULTANTS LIMITED

Bruce Halbert

Bruce E. Halbert, M.S.
Principal

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Encl.

cc R. Holmes, NUTP

RESPONSE TO QUESTIONS raised by Mr. Robert Lemire, Whiteshell Nuclear Research Establishment, Atomic Energy of Canada Limited, in correspondence dated 1 December 1986 on the Phase III Probabilistic Assessment Study.

63. Regarding equations (3.7.10) and (3.8.5), the depth of the bottom layer (λ_4) is given by:

$$\lambda_4 = 10 - (\lambda_w + \lambda_{mix})$$

as you correctly note.

64. The procedure followed in the lime added scenario involves calculating the lime inventory remaining at the end of each time step (i.e. at time = t). If the lime inventory is calculated to be depleted at any point in time, then the values for several parameters are immediately recalculated including the values of the parameters KRATE and SFLUX.

65. Yes, the factor of 1000 should be multiplied by the entire expression in equation (3.3.69). The left-hand bracket should be moved to the right of the 1000 multiplier.

66. The differences in the exponents in some of the equations for calculating pH are due to round-off error. The correct term in equations (3.3.68) and (3.3.69) and elsewhere for:

$$\frac{10^{11.86 - 2pH}}{f} \quad \text{is} \quad \frac{10^{11.87 - 2pH}}{f}$$

Similarly, the correct term in equation (3.3.65) and elsewhere for:

$$\frac{10^{2pH - 16.46}}{f} \quad \text{is} \quad \frac{10^{2pH - 16.47}}{f}$$

To reiterate, the terms given on the right-hand side above are the correct expressions.

67. I presume you are referring to equation (3.5.5) and not equation (3.3.5). If so, you are correct to suggest that the bracket in equation (3.5.5) should precede "exp," that is the expression should read:

$$\ldots)\exp(-f_p\,\bar{P}\,\Delta t/\epsilon\,\lambda_4)\ldots\text{and not}\ldots\,\exp)(-f_p\,\bar{P}\,\Delta t/\epsilon\,\lambda_4)$$

68. Yes, the values of pH, calcium, sulphate and d (the correction factor for sulphate complexation) are solved iteratively. The iterative solution is stopped when the change in pH is less than 0.01 pH units. The order of the calculations involves: firstly, determining the sulphate contribution from pyrite oxidation; secondly, obtaining an initial estimate of the pH value using the sulphate value from pyrite oxidation; and, finally, solving for equations (3.3.38), (3.3.39), (3.3.40) and (3.6.23) interatively.

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11 December 1986

Mr. Robert Lemire
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Pinawa, Manitoba
R0E 1L0

Re: Response to Questions Regarding the UTAP Phase III Code Documentation

Dear Robert:

Attached please find our response to residual questions you raised in correspondence to us dated 5 September and 5 November 1986. As in previous correspondence we have structured our response to correspond exactly with the numerical order of the questions in your letter.

I trust our answers help clarify the questions you raised. Please feel free to call to discuss points which you find unclear.

Yours very truly,

SENES CONSULTANTS LIMITED

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Encl.

cc R. Holmes, NUTP

Specialists in Energy, Nuclear and Environmental Sciences

RESPONSE TO QUESTIONS raised by Mr. Robert Lemire, Whiteshell Nuclear Research Establishment, Atomic Energy of Canada Limited, in correspondence dated 5 September and 5 November 1986 on the Phase III Probabilistic Assessment Study.

2. Equations (4.1) and (4.2) refer to the release of radon from the unsaturated zone which is divided into two layers. The model formulation is based on the assumption that no radon is released from the underlying saturated zone. Equation (4.1) applies during early times before the unsaturated layer has been depleted of barium sulphate (and hence radium-226). Equation (4.2) applies when the thickness of the lower zone of the unsaturated layer (i.e. the layer which has not yet been depleted of radium-226) becomes less than 1×10^{-3} m thick.

   The WNRE comment refers to a draft version of Volume 3. Clearly, since the unsaturated zone is nominally a metre thick (i.e. $X_1 + X_2 = 1$) the approximation that $X_2 \rightarrow \infty$ was incorrect. The final text of Volume 3 was revised from that originally provided to WNRE.

8. The DUST model (Section 4.2) calculates the radionuclide emission rate by multiplying the emission rate of surficial tailings dust by the current radionuclide concentration of the same surficial tailings layer; this latter value is calculated in SOURCE. The radionuclides accounted for include natural uranium, total thorium (Th-232 + Th-230), lead-210 and radium-226.

   The SOIL model (Section 6.2) deposits these same radionuclides on the uppermost soil layer. However, as noted by WNRE the distinction between total thorium (Th-232 + Th-230) and thorium-232 is not maintained in Section 6.2 Since we do not distinguish between the chemical behaviour of these two isotopes, this lack of distinction does not affect the leaching and retardation calculations in SOIL. The only distinction then is the radioactive decay constant. Elsewhere in the UTAP model the radioactive decay of thorium is neglected and hence, since the chemical behaviour of the thorium isotopes is assumed to be the same, the mole fractions of total thorium which are thorium-232 and thorium-230 will remain constant. In the context of the 1000 year simulation period the radioactive decay of the thorium istopes is insignificant.

14. Unlike other UTAP models, in GSHINE it was necessary to recognize that the various uranium and thorium isotopes originate from different radioactive decay series. Moreover, in the case of uranium, the uranium parent (i.e. U-238) would not be in equilibrium with its daughters. To simplify the calculations and minimize the computer storage requirements, the following assumptions were made:

    - For deposited natural uranium, the gamma decays for the U-238 series nuclides, U-238, Th-234, Po-234 and U-234, were included. With a modelling period of 1000 years, the long half-life of the next daughter Th-230 effectively truncates the decay chain. Note that the gamma decays from Th-230 itself are not included.

    - The gamma decays from the U-235 series were neglected.

- For Ra-226, Pb-210 and Th-232, gamma decays from all daughter products down to stable lead isotopes were included on the assumption that the daughters would attain equilibrium within any particular time step. This assumption simplifies the calculation but results in somewhat conservative estimates.

59. In order to weight the air concentration by the amount of watershed area in each sector, a great deal more input information would have been necessary. Specifically, each sector containing part of the watershed would have to be specified as well as the fraction of that sector containing part of the watershed. As an alternative, a straight average was taken of the air concentrations in the sectors in which nodes were situated. Sectors in which several nodes are located were counted only once. The program also checked to ensure that sectors were not skipped in moving down the length of the watershed. If they had been, an error message describing the problem would have been generated by the program and the user would be required to divide the watershed into more, smaller segments.

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RCB-86-443

December 22, 1986

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Dear Bruce;

Thank you for your response to our previous questions.

Further to our telephone conversation last week, I am enclosing a list of questions concerning the erosion model. As discussed, some of these questions have already been answered orally, but they have been included here so there will be a written record of the responses for our documentation.

69. The distribution for "SILT" is the same for the EROSION and DUST modules, however, in the EROSION module all particles "less than 0.06mm were (considered) silt", while in DUST it is the "% of particles < 75 μm". Which is correct ?

70. What equation was used for calculation of SPRIME in the erosion model ? It could be calculated from the slope, or from the tailings area and average tailings depth. Is the angle in degrees or radians ?

71. "d" (DMID) the particle diameter in feet (eqn. 3.14.16) is listed as calculated in Table 3.6. No equation or value seems to be given. In Table 3.6 of the older draft version of SENES Vol. 3, DM "mean silt diameter", "in mm" is given as a constant 1E-2, and presumably DMID was calculated from that. Please confirm:
    DMID = 1.0E-2 / (308.4) [ft].
What is the exact conversion factor (metres to feet) used throughout the EROSION model ?

72. In the erosion model, is it correct to assume that if PH(1)>4 both at TIME=0 and at TIME=-Δt, then vegatation of the tailings pile begins at TIME=-Δt ?

73. I am unable to complete a unit check on equation 3.14.8. Which terms on the RHS have units (other than λ, which I know has units of [ft]) ?

74. The equation defining the depth of flow (DF, pg. 3-128) is not given. What is it? There is something called STORM in the old draft. Is it related ? There is no value for STORM in the current draft.

75. The selected viscosity is correct near 22°C, however, viscosity is strongly temperature dependent and will be about 50% larger at 7°C, a more reasonable average temperature for water flow over the tailings.

76. Below equation 3.14.3 λ_j seems to be defined as the sum of the lengths of the segments (to segment j), although the notation (<400′) might indicate otherwise. Certainly equation 3.14.2 would require a sum of lengths, not just the length of a particular segment. However, Table 3.6 gives λ_j (LENGTH) as the "length of slope of jth segment". Below equation 3.14.8 λ (no subscript) is described as "slope length". Which definition is correct ?

L is defined in Table 3.6 (LENGT) as "length of tailings pile". Initially I assumed this was given by the definition on page 3-124. However, on page 3-128, L is defined as the "length of flow through grassed area = λ_j". Which is correct ?

It would appear at least three different distances are used here:

1. The total length (or radius ?) of the tailings pile
2. The constant representing the length of each segment for the particular tailings pile.
3. The sum of the lengths of the segments to the bottom of any particular segment.

Which definitions and computer variable names should be used for each, and more importantly, which ones should be used in equations 3.14.2, 3.14.8 and 3.14.15 ?

Yours sincerely,

Robert Lemire

cc B. Goodwin
R.W. Holmes

7
RCB-86-06

1987-01-08

Bruce Halbert
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Dear Bruce;

Further to my telephone conversation yesterday with Colin Daniels, I am enclosing a list of questions concerning various sections of the model. As discussed, the answers to some (but not all) of these questions may be trivial, but they have been included here so there will be a written record of the responses for our documentation.

77. Am I correct in assuming that in Chapter 13 (pg 13-5) X_A is X232SA from Chapter 3, and X_W is a parameter defined by equation 3.7.29 ? The latter parameter is not defined in Table A.3, but might be X232LA.

78. There is an inconsistency in the units used for FISHC ($[F_i]_{n,t}$ in Table 11.5 and below equation 11.2. The units in Table 11.5 are probably correct.

79. Are the values of CRATHS ($[Ra_s]_t^{Th}$), THDISS ($[Th]_{diss,t}$) and THDISM ($[Th]_{diss,mix,t}$) equal to zero at t=0 or at $t=-\Delta t$?

80. According to the definition of THDISS ($[Th]_{diss,t}$) (eqn. 3.9.4) the summation sign in eqn. (3.10.26) appears to be redundant. Am I correct ? Similarly, equation (3.10.28) probably should not have a summation sign.

81. Equation (3.7.43) indicates the initial barium ion concentrations depend on the concentrations of uncomplexed sulphate ions for layers 2,3,4. For t>0, equation (3.10.9) also uses the value of the concentration of the uncomplexed sulphate ion (for layer 2) rather than WCONC(7,2,3). However, equations (3.10.33) and (3.10.39) appear to indicate that for t>0 WCONC(7,3,3) and WCONC(7,4,3) (the total sulphate concentrations) should be used. Which is correct ? Should the sulphate concentrations in

equations (3.10.33) and (3.10.39) really be calculated from terms analagous to equation (3.10.8) ? A similar problem exists for Pb-210 (see equations (3.7.53, 3.11.1, 3.11.15 and 3.11.21).

Yours sincerely,

Robert Lemire

cc B. Goodwin
R.W. Holmes

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30334

13 January 1987

Mr. Robert Lemire
Atomic Energy of Canada Limited
Whiteshell Nuclear Research Establishment
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ROE 1L0

Re: Response to Questions Regarding the UTAP Phase III Erosion Model Documentation

Dear Mr. Lemire:

Attached please find the response to questions you raised in correspondence with us dated 22 December 1986. We have structured our response to correspond with the numerical order of the questions in your letter. We suggest that the response to the last question (# 76) be read first, as this will hopefully help explain some of the points that follow. Also included at the end of the response is a clarification of three equations which, although not mentioned in your questions, we felt required additional explanation or corrections.

I trust this discussion will help clarify the points you have raised. Please feel free to call to discuss any points which you find unclear.

Yours very truly,

SENES CONSULTANTS LIMITED

Colin Daniel

Colin Daniel, B.A.Sc.
Environmental Engineer

sn

Encl.

cc. R. Holmes, NUTP

Specialists in Energy, Nuclear and Environmental Sciences

30334
13 January 1987

Response to Questions raised by Mr. Robert Lemire, Whiteshell Nuclear Research Establishment, Atomic Energy of Canada Limited, in correspondence dated 22 December 1987 on the Phase III Probabilistic Assessment Study.

69. In both the EROSION and the DUST models, all particles less than 75 µm (or 0.075 mm) were considered silt. The value of 0.06 mm reported after equation (3.14.10) should read 0.075 mm.

70. The variable "x" (or SPRIME), listed in Table 3.6, is the sine of the overall slope of the tailings pile. It is calculated as:

$$x = \sin\ (\tan^{-1}\ (S_o/100))$$

where

S_o = overall percent slope of the tailings pile

The above equation should be added to the documentation after equation (3.14.8). Also, equation (3.14.3) should be changed to read:

$$S = \frac{0.43 + 0.30\ S_o + 0.043\ S_o^2}{6.613}$$

The variables "x", "x_j" and "θ" should be removed from the equation.

71. The conversion factor (metres to feet) used in the EROSION model is: 1 ft = 0.3048 m. The following equation, used to convert the particle diameter from millimetres to feet, should be added to the documentation after equation (3.14.16):

$$d = d_m/(304.8\ \text{mm.ft}^{-1})$$

where

d_m = particle diameter (mm)

The variable "d_m" should be included in Table 3.6 as:

Symbol: d_m
Description: metric mean silt diameter
Units: mm
Nominal value: 0.01
Probability distribution: C(0.01)
Computer origin: INPUT
Computer symbol: DM

72. Although the pH of the tailings surface layer may be above 4.0 at TIME = -Δt, the EROSION model assumes that revegetation will not occur before TIME = 0.

73. In order to define the units for the variables of equation (3.14.8), a corrected version of the equation is required, which is as follows:

$$T_{Cj} = rRT\lambda^2_{Cj} (x)^B C_{ro} C_T$$

T_{Cj} = bedload transport capacity for segment j (lb/ft-width/year)

r = (as before). Units are (ft^2/ (sec.yr)/"R.units")
R = USLE erosivity factor (100(ft.tons/acre)(in.hr))
T = (as before). (lb.sec/ft^5)
λ_{Cj} = length from the top of the slope to the bottom of the jth segment (ft)
x = (as before). (-)
B = (as before). (-)
C_{ro} = (as before). (-)
C_T = (as before). (-)

74. The equation for calculating the depth of flow (d_f) in equation (3.14.15) is missing from the documentation. It is as follows:

$$d_f = \frac{S_t\ L}{V\ (2.633 \times 10^7\ \text{mm.d}^{-1}/\text{ft.sec}^{-1})}$$

where

S_t = 24-hour rainfall for a 2-year return period (mm.d^{-1})
L = length of the tailings pile (ft)
V = flow velocity through the grass (ft.sec^{-1})

The variable "S_t", corresponding to the computer symbol "STORM", is missing from Table 3.6 and should be included as:

Symbol: S_t
Description: 24-hour rainfall for a 2-year return period
Units: mm.d^{-1}
Nominal value: 42
Probability distribution: U(36,48)
Computer origin: INPUT
Computer symbol: STORM

75. Correct, 7°C is a more reasonable average temperature for water flow over the tailings. The kinematic viscosity of equations (3.14.15) and (3.14.16) should be changed to $1.5 \times 10^{-5}\ \text{ft}^2.\text{sec}^{-1}$.

76. To clear up the confusion over the different lengths used in the EROSION model, here are three definitions:

L = total length of the tailings pile (ft)
= LENGT
λ_j = the length of the jth segment (where all segments are calculated to have the same length) (ft).
= LENGTH

λ_{Cj} = the length from the top of the first segment to the bottom of the jth segment (ft).

= LENTOT

The following is a list of changes to be made to the documentation. Equations (3.14.8)[1] and (3.14.15)[2] are discussed in the responses to questions 73 and 74, respectively.

(a) The variable "λ_{Cj}" should be included in Table 3.6 as:
Symbol: λ_{Cj}
Description: length from top of tailings pile to bottom of jth segment
Units: ft
Nominal value: specified in code
Probability distribution: specified in code
Computer origin: EROS
Computer symbol: LENTOT

(b) Equation (3.14.2) should read:

$$D_j = 0.0459\ RK_j\ CPS\ (\lambda_{Cj}^{m+1} - \lambda_{Cj-1}^{m+1})/72.6^m$$

Note also that the variables "CP_j" and "S_j" should read "CP" and "S", respectively, throughout the documentation, as they are independant of the segment number. In Table 3.6, "CP" should be described as the "control practice factor."

(c) At the end of Section 3.14.4 (Tailings Geometry), the following equations should be included:

$$\lambda_j = \frac{L}{N}$$

where

λ_j = length of segment j (ft)
L = total length of tailings pile (ft)

N = number of segments

$$L = (A_T)^{0.5}/(0.3048\ \mathrm{m.ft}^{-1})$$

where

A_T = surface area of the tailings (m^2)
N = INT(L/400 ft) + 1

(d) The variable "N" should be added to Table 3.6 as:

Symbol: N
Description: number of segments
Units: -
Nominal value: specified in code
Probability distribution: specified in code
Computer origin: EROS
Computer symbol: NLEN

(e) As the tailings pile is assumed to be square, the total width is equivalent to the total length (L). This explains the "L" term in equation (3.14.21), which in fact represents the width of the tailings pile.

Other Clarification

The following is a short list of changes to the EROSION model not covered in the preceding responses:

(a) In equation (3.14.4), the soil permeability class (c) was set to 5 (for tailings).
(b) Equation (3.14.7) should read:

$$F_V = 1 - \exp\left(-\lambda_T\left((T-T_V) - \frac{\Delta T}{2}\right)\right)$$

If $F_v > 0.9$ then $F_v = 0.9$
If $T = T_v$ then $F_v = 0$

(c) In equation (3.14.14), the transport capacity equations for different slopes are reversed and should read:

$$C_T = 1.14\, V_R^{18.98} \qquad S_o \leq 0.75$$
$$C_T = 1.12\, V_R^{9.27} \qquad 0.75 < S_o \leq 1.5$$
$$C_T = 1.08\, V_R^{6.7} \qquad 1.5 < S_o \leq 2.5$$

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RCB-87-22

1987-01-21

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Dear Bruce;

Here are the written versions of the questions I have telephoned you about over the last couple of weeks. The answers you sent concerning the erosion model have been received and are most helpful

82. Is SUMBAR=0 AT t=0 or t=-Δt?

83. In equation (3.11.12) is the term $[Ra_L]_4$ equal to WCONC(4,4,3) or WCONC(4,4,2) ?

84. What are the distance values used for the division of the sectors into 5 portions. Figure 2.2 suggests 10km rings centred at 5.0,15.0 25.0 etc. Figure 10.5 suggests 3.0,5.0,10.0,20.0,50.0 as ring distances. The latter looks more reasonable. Does this mean receptor distances are 2.0km, 4.0km, 7.5km, 15km and 35km from the centre of the tailings pile ? From comments you have made on the telephone, I understand the first ring runs from 1km to 3km.

85. In Table 5.2 are the x values in the column headings real or effective distances (i.e., x or $x+x_o$) ?

86. What averages are sampled for the wind ? In your letter of September 11 you talk about a twenty year average, then about twenty ten-year averages. What was actually used. Was the same average used in all runs? Is this a user specified parameter different for each time interval in a given run ?

87. In your answer to my question 59 you talk about sectors. Do you mean sectors or area segments (i.e. divided by the rings?)

88. Are segments 11-1,10-2,9-3,9-4,9-5 the only ones considered to comprise the watershed area ??

89. In the AIR DISPERSION MODEL average values are calculated for the watershed and the total study area. This is for use later in the SOIL and VEGETATION models. However, in the SOIL model are the values for the soil K_d's sampled independently at each location ? If so, are the concentrations of the radionuclides in the second soil layer of these areas averaged for use in the VEGETATION model, or is there simply an independently sampled value for each nuclide Kd applied to each of these larger areas ?

90. In the erosion model, the calculations of the transported sediment and bedload have been described by a flow diagram rather than equations. Is the following analysis correct ?
1) calculate the sediment available for transport in the segment using equation 3.14.20 (We have defined this as SUSS(j))
2) calculate the bedload for the segment from the equation below equation 3.14.20 (We have defined this as BEDS(j), where BEDS(j)=ESOIL(j)-SUSS(j))
3) calculate SUS(j) from:
   SUS(j)=(SUS(j-1) + SUSS(j)) * (1-TRSED)
4) calculate BED(j) from:
   BED(j)=TCSOIL(j) if TCSOIL(j) < (BEDS(j) + BED(j-1))
   otherwise BED(j)=BEDS(j) + BED(j-1)

91. What equation was used in the SOIL module to calculate SOILCN used in the GROUNDSHINE module ? Was it SOILCN = ZTOT x DSOIL or ??

92. Several months ago I asked about input energy level data for the Groundshine model. In addition to other information, you sent a set of energies in each energy level for each radionuclide, and a table of the number of decays in each energy level for each radionuclide. The text (pg. 7-6 and 7-7) implies that the original input data were more complicated, requiring detail about the decays in each decay chain, but this is not a problem in itself. However, equations (7.8) and (7.9) require the "number of decays in the jth energy band for radium (only". (Figure 7.2 does not contain Ra-226, and I assume you mean Figure 7.1). Does this mean, for example:

$$N_{T1}^{Ra} = N_{Ra1} + N_{Rn1}(1.-E)$$
$$= 1.46E12 + 1.46E12\ (1-EMFRAC)$$

and $E_1^{Ra} = (1.86E-1 \times 1.46E12 + 4.7E-2 \times 1.46E12)/N_{T1}^{Ra}$

i.e., Are the energy level and decay chain values given for "RA" the values for radium only, not for the entire chain, while those for "U,TH,PB,RN" are for the entire U-238 (to Th-230), Th-232, Pb-210 and Rn-222 decay chains?

93. As both RHOS(1) and RHOS(2) in the SOIL and GROUNDSHINE models are dry densities (your letter 1986-10-15), why do they differ by approximately a factor of 10 ??

94. I assume there the concentrations of calcium and sulphate in the watershed are not considered to be directly affected by erosion of the tailings pile.

95. Just to be certain we are using the same equations, is the concentration of natural uranium at watershed node 1 represented correctly by:

$$\frac{\mathrm{WCONC(1,3,3)} \times \mathrm{SFLOW} + \mathrm{GWATC(U)} \times \mathrm{VSR} + \dfrac{10^3\mathrm{EROTOT} \times \mathrm{CONC(1,1,1)}}{\mathrm{DT} \times \mathrm{RHOTAL}}}{\mathrm{FLOWQ(1)}}$$

and the sulphate concentration at watershed node 1 by:

$$\frac{\mathrm{SFLOW} \times \mathrm{WCONC(7,3,3)} + \mathrm{VSR} \times \mathrm{WCONC(7,4,3)} + \mathrm{WATCAB} \times (\mathrm{FLOWQ(1)} - \mathrm{SFLOW} - \mathrm{VSR})}{\mathrm{FLOWQ(1)}}$$

96. On page 10-28, I believe that in the equation for $Z_{i,i}$ the first minus sign should apply only to the first term, not the entire expression. Is this correct ?

Yours sincerely,

Robert Lemire

cc B. Goodwin
R.W. Holmes

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30334

27 January 1987

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Whiteshell Nuclear Research Establishment
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Re: Response to Questions Regarding the UTAP Phase III Documentation

Dear Mr. Lemire:

Attached please find the response to questions you raised in correspondence with us dated 8 January 1987. We have structured our response to correspond with the numerical order of the questions in your letter. As well, further comments on questions asked previously on the erosion model are provided as a separate addendum.

I trust this discussion will help clarify the points you have raised. Please feel free to call to discuss any points which you find unclear.

Yours very truly,

SENES CONSULTANTS LIMITED

Bruce E Halbert

Bruce E. Halbert, M.Sc.
Principal

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Encl.

cc. R. Holmes, NUTP

Specialists in Energy, Nuclear and Environmental Sciences

Response to Questions raised by Mr. Robert Lemire, Whiteshell Nuclear Research Establishment, Atomic Energy of Canada Limited, in correspondence data 8 January 1987 on the Phase III Probabilistic Assessment Study.

77. Yes, you are correct in assuming that the parameters X_A and X_W, discussed on page 13-5 of Volume 3, are given by equations (3.7.30) and (3.7.29), respectively. The equivalent computer symbols for these parameters are:

X_A = X232SA

X_W = X232LA

As noted, the latter parameter is not included in Table A.3.

78. Yes, the units of the parameter FISHC(i,n) are correctly given as $Bq.g^{-1}$ in Table 11.5. The units stated for the parameter below equation (11.2) are incorrect.

79. The concentrations of the parameters CRATHS, THDISS and THDISM are initialized to 0.0 $mol.m^{-3}$ at time $t = -\Delta t$.

80. If you treat the parameters $[Th]_{diss,t}$ and $[Th_L]_{diss,t}$ as being equivalent, then you are correct in assuming that the summation sign is redundant in equation (3.10.26). However, these two parameters have been defined slightly differently and the summation sign is thus required. The same argument holds for equation (3.10.28).

81. The influence of the uncomplexed sulphate ion on the dissolution of barium sulphate and lead sulphate is accounted for only in the unsaturated layer in the UTAP code. The rationale for taking into account the influence of uncomplexed sulphate in the unsaturated layer only is that the effect is negligible in the saturated layer where the pH is higher and the dissolved iron is reduced to the ferrous state. Hence, equations (3.10.9), (3.10.33), (3.10.39), (3.11.1), (3.11.15) and (3.11.21) are correct as stated. Equations (3.7.43) and (3.7.53) on the other hand are misleading. The subscript "ℓ" for layer number should be

replaced by "λ_W" in these equations as they only apply to layer 2. The basic structure of equations (3.7.43) and (3.7.53) is applicable to calculating the liquid phase barium and lead concentrations, respectively, in layers 3 and 4 provided the term for uncomplexed sulphate ($[SO_4^{2-}]_{u,\ell}$) is replaced by the parameter for total sulphate (i.e. WCONC (7,3,3) for layer 3 or WCONC (7,4,3) for layer 4).

. Further Clarification to questions raised by Mr. Robert Lemire, Whiteshell Nuclear Research Establishment, Atomic Energy of Canada Limited, on the UTAP Phase III Erosion Model Documentation.

(a) In equation (3.14.2), the slope exponent (m) should be calculated as:

$m = 0.3$	$S_0 \leq 3$
$m = 0.4$	$3 < S_0 < 5$
$m = 0.5$	$S_0 \geq 5$

(b) Equation (3.14.11) should read:

$$B = 1.83\ D_{50}^{0.049} \qquad 0.016 \leq D_{50} < 0.045$$

$$B = -0.714\ D_{50} + 1.61 \qquad 0.045 \leq D_{50} \leq 0.215$$

(c) In equation (3.14.14), the range for S_0 of: $1.5 < S_0 \leq 2.5$ should be changed to: $S_0 > 1.5$

(d) The text preceding the suspended sediment transport equation (3.14.15) states that "no suspended sediment is trapped when the soil is bare". Although the fraction of sediment trapped will be less when the soil is bare, some sediment will still be trapped. Also, the length term "L" in equation (3.14.15) should be replaced with the segment length "λ_j". It should also be noted that the expression on the right-hand side of equation (3.14.15) is part of the exponent, that is

$$T_r = \exp\left\{(-1.05 \times 10^{-3}) \left[\frac{VR_s}{\nu}\right]^{0.82} \left[\frac{\lambda_d}{Vd_f}\right]^{-0.91}\right\}$$

(e) Equation (3.14.20), should read:

$$E_{sj} = E_{sj-1} + D_j\ (\%\ \text{silt}/100)\ (1 - T_r)$$

$$E_{Bj} = E_{Bj-1} + D_j - E_{sj}$$

If $E_{Bj} \geq T_{cj}$ then $E_{Bj} = T_{cj}$

where:

E_{sj} = suspended sediment load leaving segment j (lb/ft-width/yr)
E_{Bj} = bedload leaving segment j (lb/ft-width/yr)
D_j = soil detached in segment j (lb/ft-width/yr)
T_r = fraction of suspended sediment trapped
T_{cj} = bedload transport capacity for segment j (lb/ft-width/yr)

(f) In calculating the depletion of the tailings pile at time t, equation (3.14.22) should read:

$$[D_T]_t = [D_T]_{t-\Delta t} + \frac{T_m\ (1000\ g.kg^{-1})}{\rho\ A_T}$$

(g) In Table 3.6, the variables E_B and E_s should be E_{Bj} and E_{sj}, respectively, as they represent the load leaving segment j.

RCB-87-36

1987-01-29

Bruce Halbert
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Dear Bruce;

A few more questions.

97. Section 9.4 and Figure 9.3 indicate the time intervals needed for equation (9.15) begin at TIME=0 (i.e., $t_o=0$). Is this correct or is $t_o=-\Delta t$?

98. Did your response (1987-01-27) to my question 80. also mean that
$\Sigma[Th_L]_{diss,t} \neq [Th]_{diss,t}$?
If so, where and how are $[Th_L]_{diss,t}$ and $[Th_L]_{diss,mix,t}$ defined ? They do not seem to be explicitly defined in section 3.9 nor Appendix A.3

99. I thought I understood how X232SA on page 13-5 was calculated. After your answer to my question 77 I am no longer as certain. I think X_A (X232SA) is calculated from equation (3.9.11). Equation (3.7.30) only gives the initial value. Am I correct ?

100. Is λ_d in the equation (given in "Further Clarification (d) in your letter of 1987-01-27) to replace equation (3.14.15) defined by:
$\lambda_d = \lambda_j \times V_s$?

Yours sincerely,

ORIGINAL SIGNED BY

Robert Lemire

cc B. Goodwin ✓
R.W. Holmes

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30334-7

3 February 1987

Mr. Robert Lemire
Atomic Energy of Canada Limited
Whiteshell Nuclear Research Establishment
Pinawa, Manitoba
ROE 1LO

Re: Response to Questions Regarding the UTAP Phase III Documentation

Dear Mr. Lemire:

Attached please find the response to questions you raised in correspondence with us dated 21 and 29 January 1987. We have structured our response to correspond with the numerical order of the questions in your letter. I believe the attached completes the responses owing on questions raised to date.

I trust this discussion will help clarify the points you have raised. Please feel free to call to discuss any points which you find unclear.

Yours very truly,

SENES CONSULTANTS LIMITED

Bruce E Halbert

Bruce E. Halbert, M.Sc.
Principal

ls

Encl.

cc. R. Holmes, NUTP

Specialists in Energy, Nuclear and Environmental Sciences

Response to Questions raised by Mr. Robert Lemire, Whiteshell Nuclear Research Establishment, Atomic Energy of Canada Limited, in correspondence dated 21 January and 29 January 1987.

82 The parameter SUMBAR is equal to zero at time $t = -\Delta t$.

83 The parameter $[Ra_L]_4$ in equation (3.11.12) is equal to WCONC (4,4,3).

84 The radial distances used in the generic assessment are 3.0, 5.0, 10.0 20.0 and 50.0 km as suggested on Figure 10.5. As noted in our documentation, the inner distance starts at 1.0 km. The program calculates the air concentration at the mid-point of each concentric ring, that is, at distances of 2.0, 4.0, 15.0 and 35.0 km from the centre of the tailings area in each of the 18 directions from the site.

16

85 The x values in Table 5.2 in the column headings are real distance x (not $x+x_0$).

86 The twenty year average was used for all the runs. the twenty ten-year averages are available if the user wishes to treat wind as a time-variant parameter. The user specifies the name of the wind data file to be used in INPUT2.DAT.

87 In our response to question 59, the term "sector" should be replaced by "area segment" as you correctly note.

88 Yes, the only area segments considered to comprise the watershed are 11-1, 10-2, 9-3, 9-4, and 9-5.

89 In the soil model, the parameter K_d is sampled once each trial for each radionuclide and applied to all segments. Because there is a lack of adequate information to distinguish between the K_d values each soil layer, the same sampled value is applied to layer 1, layer 2, and layer 3 during each trial.

90. Equation (3.14.20) should read as follows:

$$E_{sj} = [E_{sj-1} + D_j\ (\%silt/100)]\ (1-T_r)$$

$$E_{Bj} = E_{Bj-1} + D_j\ [1-(\%\ silt/100)]$$

$$\text{If } E_{Bj} \geq T_{cj} \text{ then } E_{Bj} = T_{cj}$$

The equations you have indicated are correct with suspended sediment available calculated as:

SUSS (J) = ESOIL (J) * (SILT/100)

The equations indicated under item e) in our correspondence to you dated 27 January 1987 should be disregarded.

91. The equation used in the soil module to calculate SOILCN as used in the groundshine module is SOILCN = ZTOT/DSOIL.

92. Yes, your interpretation of the number of decays in the first energy interval for radium-226 plus radon daughters which have not escaped from the soil is correct.

The total gamma ray energy spectrum from 0 to 3 MeV has been divided into five intervals 0-0.2, 0.2-0.43, 0.43-0.61, 0.61-1.4 and >1.4 MeV (see attached table).

The average energy and the average number of gamma rays emitted per second into each of the five energy intervals have been calculated for each of five radionuclide groups. The five radionuclides groups are:

```
UTAP2

Number of gamma rays per kg per second in each energy interval
for each radionuclide group

energy interval        1         2         3         4         5

radionuclides
in group

U238-U234         9.60E+05 0.00E+00 0.00E+00 1.26E+05 0.00E+00
Th232-Pb208       1.45E+05 2.79E+06 1.58E+06 2.27E+06 1.52E+06
Pb210             1.20E+14 0.00E+00 0.00E+00 0.00E+00 0.00E+00
Ra226             1.46E+12 0.00E+00 0.00E+00 0.00E+00 0.00E+00
Rn222-Pb206       1.46E+12 2.01E+13 1.72E+13 6.23E+12 6.22E+12


Average energy (Mev) in each energy interval for each radionuclide group

energy interval        1         2         3         4         5

radionuclides
in group

U238-U234         7.90E-02 0.00E+00 0.00E+00 9.10E-01 0.00E+00
Th232-Pb208       5.96E-02 2.63E-01 5.67E-01 9.00E-01 2.57E+00
Pb210             4.70E-02 0.00E+00 0.00E+00 0.00E+00 0.00E+00
Ra226             1.86E-01 0.00E+00 0.00E+00 0.00E+00 0.00E+00
Rn222-Pb206       4.70E-02 3.31E-01 6.09E-01 1.12E+00 1.76E+00


          Mass absorption coefficient for tissue m2/kg

energy interval        1         2         3         4         5

                     0.003     0.003     0.003     0.003     0.003



          Specific activity of each radionuclide in Bq/kg

          U238     Th232    Pb210    Ra226
          1.23E+07 4.03E+06 3.00E+15 3.66E+13
```

1) U238 to U234 inclusive (assuming equilibrium)
2) Th232 to Pb208 inclusive (assuming equilibrium)
3) Pb210 only
4) Ra226 only
5) Rn222 to Pb206 inclusive (assuming equilibrum)

One of the first computational steps is to calculate the combined contributions to total gamma radiation from Ra226 (group 4) and radon daughters (group 5) which have not escaped from the soil. In your question you correctly described this calculation for the first energy interval.

93. The densities of soils comprising layer 1 and layer 2 in the soil model differ by a factor of ten because layer 1 represents an organic mat whereas layer 2 consists primarily of inorganic minerals. The organic mat is characteristic of the forested areas covering the Precambrian Shield. This distinction would not apply, of course, if one were modelling a facility located in a developed area, such as in Southern Ontario.

94. Correct, the leachable precipitates are considered to have been previously dissolved from tailings solids removed from the surface of the tailings area by surface erosion.

95. The correct equation for calculating natural uranium at watershed node 1 is:

$$\mathrm{WATC}(1,1,3) = [\mathrm{WCONC}(1,3,3) \times \mathrm{SFLOW} + \mathrm{GWATC}(1,3) \times \mathrm{VSR}]$$

$$\times \frac{[\mathrm{EROTOT} \times 1000 \times \mathrm{CONC}(1,1,3)]}{\mathrm{DT} \times \mathrm{RHOTAL}} \times \frac{1}{\mathrm{FLOWQ}\ (1)}$$

The correct equation for calculating the sulphate concentration at node 1 is:

$$\mathrm{WATC(7,1,3)} = [\mathrm{WCONC(7,3,3)} \times \mathrm{SFLOW} + \mathrm{WTSO4B} \times (\mathrm{FLOWQ(1)}-\mathrm{SFLOW})] \times \frac{1}{\mathrm{FLOWQ(1)}}$$

The contribution of the groundwater component to sulphate (and calcium) is assumed to be equal to the natural background level and thus is not explictly included in the calculation.

96. Yes, the minus sign applies only to the first term, not the entire expression, in the equation for $Z_{1,i}$ on page 10-28.

97. The subsurface transport model calculations begin at time t = 0 years.

98. No, it was intended that you would interpret that $\Sigma[TH_L]_{diss,t} = [Th]_{diss,t}$. The difference between the two parameters is that the former parameter gives the instantaneous concentration at time 't' whereas the latter gives cummulative mass per unit volume dissolved to time 't'. The definition given by equation (3.9.4) holds.

99. You are correct. The initial value of the parameter X_A(X232A) is given by equation (3.7.29). The value of the parameter X_A at any other time (i.e. X232SA) is given by equation (3.9.11).

100. As suggested, the parameter λ_d in the revised version of equation (3.14.15) replaces $\lambda_j\ V_s$. However, this was not intended. Instead the equation should read:

$$T_r = \exp\ (-1.05 \times 10^{-3})\ \underline{VR_s}^{\,0.82}\ \left(\frac{\lambda_j V_s}{Vd_f}\right)^{-0.91}$$

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30334-7

4 February 1987

Mr. Robert Lemire
Atomic Energy of Canada Limited
Whiteshell Nuclear Research Establishment
Pinawa, Manitoba
ROE 1L0

Re: Response to Questions Regarding the UTAP Phase III Documentation

Dear Mr. Lemire:

Please find enclosed a replacement copy for the last page of the material sent to you yesterday. In our haste to get it out in time to make the courier service, we inadvertently left the brackets off the equation discussed under item 100.

Yours very truly,

SENES CONSULTANTS LIMITED

Bruce E. Halbert

Bruce E. Halbert, M.Sc.
Principal

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Encl.

$$\mathrm{WATC}(7,1,3) = [\mathrm{WCONC}(7,3,3) \times \mathrm{SFLOW} + \mathrm{WTSO4B} \times (\mathrm{FLOWQ}(1)-\mathrm{SFLOW})] \times \frac{1}{\mathrm{FLOWQ}(1)}$$

The contribution of the groundwater component to sulphate (and calcium) is assumed to be equal to the natural background level and thus is not explictly included in the calculation.

96. Yes, the minus sign applies only to the first term, not the entire expression, in the equation for $Z_{1,i}$ on page 10-28.

97. The subsurface transport model calculations begin at time t = 0 years.

98. No, it was intended that you would interpret that $\Sigma[TH_L]_{diss,t} = [Th]_{diss,t}$. The difference between the two parameters is that the former parameter gives the instantaneous concentration at time 't' whereas the latter gives cummulative mass per unit volume dissolved to time 't'. The definition given by equation (3.9.4) holds.

99. You are correct. The initial value of the parameter X_A(X232A) is given by equation (3.7.29). The value of the parameter X_A at any other time (i.e. X232SA) is given by equation (3.9.11).

100. As suggested, the parameter λ_d in the revised version of equation (3.14.15) replaces $\lambda_j V_s$. However, this was not intended. Instead the equation should read:

$$T_r = \exp\left\{(-1.05 \times 10^{-3})\left[\frac{VR_s}{\nu}\right]^{0.82}\left[\frac{\lambda_j V_s}{Vd_f}\right]^{-0.91}\right\}$$

Notes from a call to SENES; 1987 February 17
(B.W. Goodwin, C. Hallam)

A comparison of the input files for UTAP2 and SYVAC3-UT2 has revealed some differences. They are:

1) UTAP2 has WYEAR and LAYER. What are they?
   Answer:
   WYEAR is a file selection parameter. It is sampled from a uniform pdf with a range of 1 to 20, and used to select wind data from one of 20 input files (each file has 10-year averages for a 10-year time step, or 1-year averages for a 1-year time step).
   LAYER is (probably) the number of soil layers (=2). It is defined as NLAYER in the SYVAC3-UT2 data dictionary.

2) SYVAC3-UT2 has the following parameters, not input to UTAP2: AW, BW, BSOIL, DCFGA, DCFGW, DCFHA, ENERGY, MUFLSH, SPA and STDYAR. Are they hard-coded constants in UTAP2?
   Answer: ENERGY and SPA are definitely hard-coded. STDYAR is calculated, probably as the area of a 50 km circle. The others are probably hard-coded in.

3) We do not have a copy of the user's manuals and so cannot check all input, in particular for the first lines of DET1 and all of DET2.

C. Hallam will confirm the above answers and forward a copy of the UTAP2 user's manual to us.

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30334-7

18 February 1987

Dr. Bruce Goodwin
Atomic Energy of Canada Limited
Whiteshell Nuclear Research Establishment
Pinawa, Manitoba
ROE 1LO

Dear Bruce:

Please find enclosed a copy of the Users Manual for UTAP2. Appendix D gives definitions of all of the probabilistic input variables. I checked the origins of all of the variables that you asked about and found that they were all assigned within the program rather than as input variables.

The air dispersion coefficients, A and B are as on the attached Table 1 reproduced from Table 5.2 of Volume 3 of the Phase III report, with minor modifications.

The soil structure code (BSOIL) is assigned a constant value of 2. The dose conversion factor variables DCFGA, DCFGW and DCFHA are assigned the values given in Table 13.3 of Volume 3 except for Thorium for which these factors are calculated as described elsewhere in Chapter 13.

The following variables in the groundshine model are assigned the values indicated on the attached Table 2:

ENERG - Average energy in each energy level for each radionuclide

NNDEC - Number of decays in each energy level for each radionuclide

SPA - Specific activity for each radionuclide

MUFLSH - Mass energy adsorption coefficient for each energy band

Each ring mid point (RNGMID) is calculated as the average of the inner and outer radial distances of that ring. The total area is the area inside the outer ring less the area inside the inner ring. The area used for calculating

...2

average air concentrations for moose and caribou is taken as the sum of the areas of the sectors that have one or more watershed end nodes located in them.

If you have any further questions, please don't hestitate to call me.

Yours very truly,

SENES CONSULTANTS LIMITED

Cecile E. Hallam, B.A. Sc.
Environmental Engineer

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Encl.

Table 1

POWER LAW EXPONENTS AND COEFFICIENTS FOR σ_Z

Atmospheric Stability Class	Downwind Distance meters $500 < x < 5000$		Downwind Distance meters $5000 < x < 50,000$	
	a	b	a	b
A	0.0002539	2.086	0.0002539	2.089
B	0.04936	1.114	0.04936	1.114
C	0.1014	0.9260	0.1154	0.9109
D	0.2591	0.6869	0.7368	0.5642
E and F	0.2017	0.6020	1.5763	0.3606

Notes:

1) $\sigma_Z = a(x+x_0)^b$

2) In this application if σ_Z is predicted to be greater than 5000m, σ_Z is set equal to 5000m

3) Stability classes E and F are represented by coefficients for class F.

4) Coefficients a and b are from CDM (1973 p. 8).

Table 2

CONSTANT VALUES FOR GROUNDSHINE

a) Average Energy (MeV)

Radionuclide	Energy Band				
	1	2	3	4	5
Uranium	7.9×10^{-2}	0	0	9.1×10^{-1}	0
Thorium	5.96×10^{-2}	2.63×10^{-1}	5.67×10^{-1}	9.00×10^{-1}	2.57
Lead	4.7×10^{-2}	0	0	0	0
Radium	1.86×10^{-1}	0	0	0	0
Radon	4.7×10^{-2}	3.31×10^{-1}	6.09×10^{-1}	1.12	1.76

b) Number of Gamma Decays (gamma.kg^{-1}.s^{-1})

Radionuclide	Energy Band				
	1	2	3	4	5
Uranium	9.55×10^{5}	0	0	1.26×10^{5}	0
Thorium	1.45×10^{5}	2.795×10^{6}	1.58×10^{6}	2.27×10^{6}	1.52×10^{6}
Lead	1.2×10^{14}	0	0	0	0
Radium	1.46×10^{12}	0	0	0	0
Radon	1.46×10^{12}	2.01×10^{13}	1.72×10^{13}	6.23×10^{12}	6.22×10^{12}

c) Specific Activity (Bq.kg^{-1})

Radionuclide	
Uranium	1.23×10^{7}
Thorium	4.03×10^{6}
Lead	3.00×10^{15}
Radium	3.66×10^{13}

d) Mass Energy Adsorption Coefficient (m^{2}.kg^{-1})

Energy Band	
1	3.0×10^{-3}
2	3.0×10^{-3}
3	3.0×10^{-3}
4	3.0×10^{-3}
5	3.0×10^{-3}

Notes on Remaining Questions

101. DSOIL assumed to be the soil layer thickness, not depth. (RJL)

102. in question 92. I wrote

$$N_{T1}^{RA} = N_{Ra1} + N_{RN1}(1.-E)$$
$$= 1.46E12 + 1.46E12\ (1-EMFRAC)$$

and $E_1^{Ra} = (1.86E-1 \times 1.46E12 + 4.7E-2 \times 1.46E12)/N_{T1}^{Ra}$ and you said this was right. However I think I should have had the term 4.7E-2 x 1.46E12 in the last equation multiplied by (1-EMFRAC). Am I now correct? (RJL)

103. The data you supplied for the first energy interval (number of γ-rays and average energy) are different in your letters of (1986-10-15 and 1987-02-03). I assume the latter set is correct. (RJL)

104. It has been assumed the total groundshine dose is the sum of the doses from the separate decay chains. Is this correct? Should the dose be the total groundshine dose multiplied by the occupancy factor (OF) of Chapter 13? (RJL)

105. Am I correct to assume WATC(nuc,n)=WATRW(nuc,n)=WATRC(nuc,n)=0 at t=0 for all radionuclides? (RJL)

106. At one time you sent an equation for parameter FWINDT1 that does not seem to appear in the documentation. Where is it used (or is it used at all)?
FWIND1(d) FRACTION OF TIME WIND BLOWS TO RECEPTOR WITH HIGH WIND SPEEDS [-]. Fraction of the time the wind blows from the tailings source to the receptor (a 'critical' man or vegetation) (i.e., in a particular direction, with high wind speeds (velocities > 5.4 $m \cdot s^{-1}$). Used in the ? module and calculated from STAR data using an equation supplied in a letter by SENES (1986-11-04):

$$FWINDT1 = \sum_{s=1}^{6} \sum_{v=4}^{6} FWIND(d,s,v,n) \quad (RJL)$$

107. I assume CALIME = 0 when INLIME($t-\Delta t$)=0, by definition of the calcite option. (BWG)

108. Inspection of the UTAP2 code shows the initial condition for WCONC(6,2,3) is as in eqn. (3.3.14) except the factor 0.1 is omitted. (BWG)

109. Inspection of the UTAP2 code shows that WCONC(7,1,3)=0 at t=0. (BWG) The model should probably have it set equal to WTSO4B. (BWG)

110. Inspection of the UTAP2 code shows that DGYP=0 at t=0. (BWG)

111. Inspection of the UTAP2 code shows that CONC(1,1,3)=CONC(1,1,1) at t=0. (BWG)

112. Inspection of the UTAP2 code shows that THDISS=0 at t=0. (BWG)

113. Inspection of the UTAP2 code shows that CRATHS=0 at t=0. (BWG)

114. Inspection of the UTAP2 code shows that CONC(4,1,3)=CRADTI * RACF at t=0. (BWG)

115. Inspection of the UTAP2 code shows that CONC(4,2,3)=CRADI * RACF at t=0. (BWG)

116. Inspection of the UTAP2 code shows that WCONC(4,3,3) has the initial condition shown in DDD 1.4.4.5. (BWG)

117. Inspection of the UTAP2 code shows that WCONC(3,2,3) has the initial condition shown in DDD 1.5.2.7. (BWG)

118. I assume that SUMPB(-Δt)=0. (BWG)

119. I assume that WCONC(3,3,2)=0 at t=0. (BWG)

120. Inspection of the UTAP2 code shows that WCONC(3,4,3) has the initial condition shown in DDD 1.5.3.8. (BWG)

121. I assume that WCONC(3,4,2)=0 at t=0. (BWG)

122. Inspection of the UTAP2 code shows that WCONC(3,3,3) has the initial condition shown in DDD 1.5.3.5. (BWG)

123. Inspection of the UTAP2 code shows that CPBRAS=0 at t=0. (BWG)

124. Inspection of the UTAP2 code shows that WCONC(4,2,3) has the initial condition shown in DDD 1.4.3.5. (BWG)

125. Inspection of the UTAP2 code shows that WCONC(4,4,3) has the initial condition shown in DDD 1.4.4.8. (BWG)

126. Inspection of the UTAP2 code shows that, in the calculation of PH2, the variable WCONC(6,2,3) was used instead of WCONC(7,2,3), and that the factor $10^{8.97}$ was used instead of $10^{8.99}$. Similar problems exist in the calculation of PH1. (BWG)

127. Inspection of the UTAP2 code shows that eqn. (3.9.16) must be modified by factors of 1000 [dm^3m^{-3}] wherever WCONC(7,3,3) occurs. (BWG). This problem appears in DDDs 1.3.2.6A and 1.3.2.8.

128. Inspection of the UTAP2 code shows that UWIND(dir,st) has a minimum value of 0.5. (BWG)

129. Inspection of the UTAP2 code shows that AIRC(nuc,loc) should be modified as shown in DDD 2.3.5. The equation for FWIND1 was supplied by SENES in a letter dated 86-11-04. (BWG)

130. Inspection of the UTAP2 code shows that RNGMID is not an input parameter, but calculated from RL (see DDD 2.3.3). The latter is a new input parameter. (BWG)

131. Inspection of the UTAP2 code shows that RAREA and TAREA must be calculated as shown in DDD 2.3.7A. Furthermore, the corresponding equations for AIRC(nuc,81) and AIRC(nuc,82) must be modified as shown in DDD 2.3.6 and 2.3.7. (BWG)

132. We note that, in the UTAP2 listing, the STAR data file is input as follows:

```
     FWIND(dir,st,vel,yr), dir = 9 to 16, then 1 to 8
                            st = 1 to 6
                           vel = 1 to 6
```

The unusual ordering for dir was unexpected; we assume the above is correct. (BWG)

133. Inspection of the UTAP2 code shows that PYRITE(t=0) is set equal to PYRITI, as well as at ($t=-\Delta t$). (BWG)

134. Inspection of the UTAP2 code shows that the factor 1.067 has been substituted for 8/7.5 in the calculation of SFLUX. (BWG)

135. Inspection of the UTAP2 code shows a logic error that sets XLEAD=0 for t>0, and CONC(3,1,3) = CPBRAS * PBCF for t>0. We have implemented both of these equations in SYVAC3-UT2. (BWG)

136. Inspection of the UTAP2 code shows that WCONC(7,1,3) is set equal to WCONC(6,1,3) both before and after gypsum is depleted in the unsaturated zone, which is inconsistent with the documentation. Since WCONC(6,1,3) is not referenced in the specifications, we have modified WCONC(7,1,3) to match the UTAP2 code (see DDD 1.1.3.1). This correction also affects the previous comment for PH1: its equations should now reference WCONC(7,1,3) as shown in the specifications (see DDD 1.1.3.2). (BWG)

137. We have assumed that FNG(nuc)=0 at t=0, and that FNG(nuc) is reset to 0 if its calculated value is less than 1.0E-30, for consistency with the UTAP2 code. (BWG)

138. Inspection of the UTAP2 code shows that GWATC(nuc)=0 at t=0. We have included this initial condition in SYVAC3-UT2. (BWG)

139. Inspection of the UTAP2 code shows that SFLOW is not subtracted from FLOWQ(1) as shown in DDDs 3.2.5 and 3.2.5A. We have adjusted SYVAC3-UT2 accordingly. (BWG)

140. Inspection of the UTAP2 code shows that, if WCONC(6,2,3)=0, it is reset to 1.0D-20. This correction was implemented in SYVAC3-UT2. (BWG)

141. Inspection of the UTAP2 code shows that BEXP should be calculated as shown in DDD 1.6.1.6, and has been implemented in SYVAC3-UT2. (BWG)

142. Inspection of the UTAP2 code shows that the logic for TVEG, FVEG and CSOIL is as shown in DDD 1.6.1.7 (see Note 4). We have implemented the changes noted into SYVAC3-UT2. (BWG)

143. Inspection of the UTAP2 code shows that a different equation for SUS was used, as noted in DDD 1.6.3.6. The new expression has been used in SYVAC3-UT2. (BWG)

144. Inspection of the UTAP2 code shows that a different equation for BED was used, as noted in DDD 1.6.3.7. The new expression has been used in SYVAC3-UT2. (BWG)

145. Inspection of the UTAP2 code shows that the equation for EROTOT, given in DDD 1.6.3.10, does not include the variable NLEN as a multiplier. It has been removed from SYVAC3-UT2. (BWG)

146. Inspection of the UTAP2 code shows that a different equation for SLPFAC was used, as noted in DDD 1.6.3.3. This different equation was used in SYVAC3-UT2. (BWG)

147. Inspection of the UTAP2 code shows that the equations for KW and KS are incorrect in the SENES documentation, and should be as noted in DDDs 3.3.8.2 and 3.3.8.3. Corrected equations are used in SYVAC3-UT2. (BWG) Inspection of the UTAP2 code also shows some variance in the logic for calculation of WATRW and WATRS. The logic used in SYVAC3-UT2 is shown in DDDs 3.3.8.10 and 3.3.8.11. (BWG)

148. Inspection of the UTAP2 code shows that a different equation was used for WSIGD for the first lake downstream from the tailings. The corrected equation, noted in DDD 3.3.5, was used in SYVAC3-UT2. (BWG)

149. Inspection of the UTAP2 code shows some variance in the logic for calculation of WATCCA and WATCS, as noted in DDD 3.2.6. The amended logic has been implemented in SYVAC3-UT2. (BWG)

150. Inspection of the UTAP2 code shows that the equations for WATCCA and WATCS are modified, as noted in DDDs 3.2.5 and 3.2.5A. These changes disagree with those given in response #95 (SENES letter dated 1987-02-03). The corresponding changes have been implemented in SYVAC3-UT2. (BWG)

151. Inspection of the UTAP2 code shows that the initial condition for X232SA is as noted on DDD 1.3.2.5C. The logic used to calculate X232SA is also somewhat different from the SENES documentation, and is noted in DDD 1.3.2.5C. SYVAC3-UT2 has been modified accordingly. (BWG)

152. Inspection of the UTAP2 code shows that the initial condition for THDISM is THDISM=0 at t=0. SYVAC3-UT2 has been modified accordingly. (BWG)

153. Inspection of the UTAP2 code shows that, in the equation for RADD on p. 13-17 of their manual, the factor 69.6 has been used instead of 6.96. Calculation of the factor shows that the former value is correct, and it has been implemented in SYVAC3-UT2. (BWG)

154. Inspection of the UTAP2 code shows that, for calculation of PH2, the terms $2 * \text{WCONC}(8,2,3) * 10^{-3}$ and $10^{-3} * \text{WCONC}(7,2,3) * \{...\}$ are modified as noted in DDD 1.1.2.8. Both modifications have been implemented in SYVAC3-UT2. (THA)
The modification previously noted in comment #126 also applies. (BWG)

155. Inspection of the UTAP2 code shows that SOILA is not included in the coded equations for BETAO (see DDDs 2.4.1 and 2.4.5), ZAVG (see DDD 2.4.4) and SOILCN (see DDD 2.4.6). Since SOILA is a constant equal to 1.0, the calculations should not be affected. (BWG)

156. Inspection of the UTAP2 code shows that the equation for BETAI (see DDD 2.4.2) is modified by the multiplicative factor (1-FWAT) for soil layers other than the topmost layer. This factor has been coded into SYVAC3-UT2. (BWG)

157. Inspection of the UTAP2 code shows that the two exponential terms in the equation for ZTOT involves the variable DT and not TIME (see DDDs 2.4.3 and 2.4.5). These two changes have been included in SYVAC3-UT2. (BWG)

158. Inspection of the UTAP2 code shows that the logic and equations for WCONC(7,1,3) are significantly different from the SENES documentation. See DDD 1.1.3.1, notes 5 to 7, for a description of the calculation of WCONC(7,1,3). (BWG)

159. Inspection of the UTAP2 code shows that there is some variation in the manner in which PH1 is calculated. See DDD 1.1.3.2 for details of the logic for calculation of PH1. (BWG)

160. Inspection of the UTAP2 code shows that KRATE can be a time-dependent variable when the lime option is used. As noted in DDD 1.1.2.3, KRATE is calculated using a new equation at the time when any added lime has dissolved. SYVAC3-UT2 has been modified accordingly. (BWG)

161. Inspection of the UTAP2 code shows that the calculation of DELTAH is different for the lime and no-lime options. The initial condition for DGYP is also shown to be zero at t=0. See DDD 1.1.2.6 for more details on the calculation of DGYP and DELTAH. (BWG)

162. Inspection of the UTAP2 code shows that WCONC(6,2,3) is reset to 1.0D-20 if its calculated value is zero. This condition has been included in SYVAC3-UT2. (BWG)

163. Inspection of the UTAP2 code shows that, in the calculation of CALIME, the factor "11.86" is used instead of "11.87". SYVAC3-UT2 has been changed accordingly.

164. Inspection of the UTAP2 code shows that the parameter DUNSAT does not appear in the calculation of INLIME (see DDD 1.1.2.5). This parameter has been removed from SYVAC3-UT2 (as part of equation (3.3.70)), in spite of the fact that the unit check now fails. We suspect that the UTAP2 code is in error. (BWG)

165. Inspection of the UTAP2 code shows that the equations for the calculation of BETA and PYRITE are modified from those given in the SENES documentation. See DDDs 1.1.2.4 and 1.1.2.1 for a description of the logic implemented in SYVAC3-UT2. (BWG)

166. Inspection of the UTAP2 code shows that there exist several differences in the equations and logic used to calculate PH2. See DDD 1.1.2.8, notes 4 to 7 for a description of the logic used in SYVAC3-UT2. (BWG)

167. Inspection of the UTAP2 code shows that WCONC(7,2,3), DELT and PH2 are not calculated iteratively. The original specifications, based on the

response to comment #68, showed that these variables were involved in a calculation loop with repeated estimations until convergence was attained. The final logic and equations for calculation of these variables are provided in their specification DDDs; see DDD 1.1.2.11 for WCONC(7,2,3), 1.1.2.9 for DELT and 1.1.2.8 for PH2. These "final" specifications are substantially different from the original documentation. (BWG)

168. Consideration of the changes above for WCONC(7,1,3) and PH1 requires modifications to several of the data flow diagrams as well. For example DFD 1.1.3 does not require the parameters DT, BETA, NPRCP and WCONC(7,2,3) for bubble 1.1.3.1, and DFD 1.1 requires related changes. Similarily, changes to the variables PH2, DELT and WCONC(7,2,3) required changes to DFDs 1.1.2 and 1.1. The final set of DFDs includes all variables in the data flows, and identifies those variables that are not actually required in the final DFDs. (BWG)

169. Inspection of the UTAP2 code shows that the equation given in response #95 (SENES letter dated 1987-03-02) are missing a set of brackets; the corrected equation is provided in DDD 3.3.6. (BWG)

170. Inspection of the UTAP2 code shows that the specifications in DDD 1.3.2.6A were missing the conversion factor 10^3 [dm^3 m^{-3}] in two places. The corresponding code in SYVAC3-UT2 was corrected. (BWG)

171. Inspection of the UTAP2 code shows that calculation of CONC(2,1,3) uses the logic as noted in DDD 1.3.2.5B. (BWG)

172. Inspection of the UTAP2 code shows that if DBAR is greater than or equal to DUNSAT, DBAR is reset to equal DUNSAT, and CBAR and MBAR are set equal to zero. SYVAC3-UT2 has been modified accordingly. (BWG)

173. Inspection of the UTAP2 code shows that WCONC(7,3,2) is used instead of WCONC(6,3,2) in the calculation of WCONC(7,3,3), based on eqn. (3.4.12). DDDs 1.1.4.4 and 1.1.4.6 are affected, and SYVAC3-UT2 was modified accordingly. (BWG)

174. Inspection of the UTAP2 code shows that XBAR is not calculated when DBAR $\geq$ DUNSAT. (BWG)

175. Inspection of the UTAP2 code revealed an error in DDD 1.1.4.1: condition (a) was changed to "If ... and DGYP $\geq$ DUNSAT ..." instead of "If ... and DGYP > DUNSAT ...". SYVAC3-UT2 was corrected accordingly. (BWG)

176. Inspection of the UTAP2 code shows that if GYPMIX(t) $\geq$ GYPI, DELTAG=0 and GYPMIX(t)=GYPI. Also, when GYPMIX(t-Δt)$\geq$GYPI, SSTAR is not recalculated but remains constant. SYVAC3-UT2 was changed accordingly. (BWG)

177. Inspection of the UTAP2 code shows that in the calculation of CIGPB, DT is used instead of TIME. (BWG)

Volume

2

WHITESHELL RESEARCH

COMPARISON OF THE NATIONAL URANIUM TAILINGS PROGRAM'S PROBABILISTIC CODE UTAP2 WITH ATOMIC ENERGY OF CANADA LIMITED'S PROBABILISTIC CODE SYVAC3-UT2

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ABSTRACT

This report describes a comparison of the output of two codes: UTAP2 (Uranium Tailings Assessment Program, Version 2) and SYVAC3 (Systems Variability Analysis Code, generation 3). Both codes are probabilistic systems assessment codes, written to serve as tools in the preparation of long-term environmental assessments. Both codes consist of a central core of 'executive' modules, to which are linked one or more submodels that are representative of the physical system being assessed.

UTAP2 has been developed for use in environmental assessments of the impact of uranium tailings.[1] Available documentation for this assessment includes a description of the model representing the tailings site. From these written descriptions, a set of model-related specifications were created, that provide a detailed description of the uranium tailings model.

The specifications were used to develop the system model code for use with SYVAC3. The resultant code, SYVAC3-UT2, was then compared with UTAP2 for three different simulations.

This report describes the steps used to prepare the specifications and prepare the tailings model code for SYVAC3-UT2. Results are also described from the comparisons of UTAP2 and SYVAC3-UT2.

NOTICE

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1/ SENES. 1986. Probabilistic Model Development for the Assessment of the Long-Term Effects of Uranium Mill Tailings in Canada - Phase III. Volume 3 - Uranium Tailings Assessment Program (UTAP) Component Model Documentation. Contract report prepared under contract #0SQ85-00182 for the National Uranium Tailings Program, Canada Centre for Mineral and Energy Technology, Energy Mines and Resources Canada, 555 Booth Street, Ottawa, Ontario, K1A 0G1.

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APPENDIX B: SPECIFICATIONS FOR THE TAILINGS MODEL

Specifications for the models in the Uranium Tailings Assessment Program (UTAP) model have been developed from the SENES Phase III Report[1]. The specifications consist of three components: data flow diagrams (DFD's), minispecifications (minispecs), and the data dictionary (DD). The following notes describe the format of the DFD's, and minispecs, and are followed by the DFD's and minispecs developed from the uranium tailing model. Notes for the data dictionary are presented in Appendix C.

Data Flow Diagrams (DFD's)

Data flow diagrams have been well described in published references (see for example DeMarco[2] and Gane and Sarson[3] The following definition of a data flow diagram comes from Page-Jones[4] :

> A DFD is a network representation of a system, and shows the active components of the system and the data interfaces between them. It is also known informally as a Bubble Chart, since it consists of little circles resembling bubbles.

The following conventions have been followed in preparing DFD's for these specifications:

(1) Circles (bubbles) represent processes, and arrows represent data flows between processes. Solid arrows represent data flows that are functions of time; dashed arrows represent data flows that are constant values. All bubbles and data flows are labelled. Bubbles are labelled with verb phrases such as "Calculate internal dose", and data flows have short unique names of up to six characters (plus optional subscript) such as DOSEIC. An asterisk next to the name of an input data flow means that the data flow enters DFD in more than one place. A bubble may have any number of incoming and outgoing data flows. If a bubble has only one outflow, such as "pH of layer 3", then the bubble name is, typically, "Calculate pH of Layer 3".

1/ SENES, 1986. Probabilistic Model Development for the Assessment of the Long-Term Effects of Uranium Mill Tailings in Canada - Phase III; Volume 3 - Uranium Tailings Assessment Program (UTAP)Component Model Documentation. Contract report prepared under contract # 0SQ85-00182 for the National Uranium Tailings Program, Canada Centre for Mineral and Energy Technology, Energy, Mines and Resources Canada, 555 Booth Street, Ottawa, Ontario, K1A 0G1.

2/ DeMarco, Tom, 1979. Structured analysis and system specification; YOURDON Inc., New York

3/ Gane, Chris and Sarson, Trish, 1979. Structured systems analysis: Tools and techniques; Prentice-Hall Inc., Englewood Cliffs, New Jersey.

4/ Page-Jones, M., 1980. The practical guide to structured systems design; YOURDON Inc., New York, p.59.

Otherwise, a more general name is used. Bubbles are also labelled with unique numeric identifiers, like "1.3.2" (the meaning of the sequence of numbers is explained below).

(2) The complete UTAP model is represented by a set of DFD's. The set contains one DFD called Figure 0 to represent the entire system at a general level. Each bubble in Figure 0 may be expanded into a full DFD representing more detailed data flows and processes. Bubbles appearing on the detailed DFD's may themselves be expanded into more detailed DFD's, recursively, until the processes are simple enough to be described by a minispec (see the next section). The bubbles are numbered to show the successive expansions. Bubbles shown in Figure 0 are numbered 1, 2, 3, etc. In Figure 1, which is an expansion of bubble 1, bubbles are numbered 1.1, 1.2, 1.3, etc. In Figure 1.1, an expansion of bubble 1.1, bubbles are numbered 1.1.1, 1.1.2, 1.1.3, etc. The lowest level of figure numbers is a minispecification design; for example figure 1.1.3.1, an expansion of bubble 1.1.3.1 in figure 1.1.3, is a minispecification figure.

(3) All variables needed in a process are shown as data flows into the appropriate bubble. All variables that are explicitly calculated must have a source bubble from which they are shown emerging. In contrast, sampled parameters are never shown emerging from a bubble; they are implicitly assumed to be produced by the SYVAC3 or UTAP2 sampling routines. Therefore, data flows shown coming from the edge of a DFD are either sampled parameters, or calculated variables that were generated on a higher level diagram. The top DFD, Figure 0, shows all the sampled parameters that are used in the model. To reduce clutter of Figure 0, these parameters are grouped together in lists. For example, bubble 1 (Calculate source term concentrations) requires several lists of parameters, including PTHS, PCHEMS and PPBS (all lists of parameters start with the prefix "P"). All such lists are defined in the data dictionary.

Minispecifications

According to DeMarco[5] a minispecification (minispec) is "a concise statement of user policy rules governing a given elemental function". Minispecs detail the workings of each process bubble that is not expanded into a DFD.

The type of minispec used for the specifications of the uranium tailings model is known as a data dependency diagram (DDD), and it contains the following components:

(1) Description of the DDD purpose. The top right corner of the DDD contains the figure number and title. The top left corner contains the short and long names and SI units of the variable (or variables) being calculated. The definition of the variable is also provided for extra information.

5/ DeMarco, Tom, 1982. Controlling software projects; YOURDON Inc., New York.

(2) Diagram showing data dependencies. A simple diagram is shown within a rectangular box. The center of the rectangle contains the variable(s) being calculated. To the left and right, respectively, are lists of the time-independent and time-dependent parameters required to perform the calculations. As in the DFD's, time-independent parameters are joined by dashed lines, and time-dependent parameters by solid lines.

(3) Description of all parameters. Below the diagram there follows a list of all parameters, including the calculated variables, that are required in this DDD. The list includes the short and long names, SI units and source of all variables. The source is either "sampled" from input sampled parameters or the number of a DDD in which the parameter is calculated.

(4) Equations: Equations are given for any calculations performed in the minispec. These equations are always referenced back to the SENES documentation, or to more recent corrections.

(5) Units check: Wherever possible, the units of equations are checked to ensure consistency. Several errors in the SENES documentation were found by the units check.

(6) Notes: Any additional explanation of the minispec is given at the bottom in the form of numbered notes.

List of Figures

There are 252 DFD's and DDD's required to specify the uranium tailings model. A list of figure numbers and their titles is given in Table B1. Table B2 gives a cross-reference of the specification DDD for each variable, followed by the complete set of DFD's and DDD's. All changes to the specifications, in particular those noted in item 21 of Appendix A, are reflected in these figures, so that these figures represent an up-to-date and final set of specifications for the SYVAC3-UT2 code.

TABLE B1 List of Specification Diagrams

Figure Number	Title	
0.0	Overview	
1.0	Calculate	Source Term Concentrations
1.1	"	pH and Calcium and Sulphate Concentrations
1.1.1	"	Time Indep. Parameters
1.1.1.1	"	Init. Gypsum Content in Tailings
1.1.1.2	"	Sq. Root of Eqbm. Const. Gypsum
1.1.1.3	"	Init. Conc. Limestone
1.1.1.4	"	Thickness Layer 4
1.1.2	Calculate	Sulphate Conc. and Other Data
1.1.2.1	"	Pyrite Conc. in Tailings
1.1.2.2	"	Sulphate Flux from Oxd'n of Pyrite
1.1.2.3	"	Rate Const. of Oxd'n of Pyrite

Table B1 cont'd

1.1.2.4	Calculate	Pyrite Oxidation Factor
1.1.2.5	"	Invent. $CaCO_3$
1.1.2.6	"	Depth of Upper Unsat. Zone
1.1.2.7	"	Ca from $CaCO_3$ Diss.
1.1.2.8	"	pH Layer 2
1.1.2.9	"	SO_4 Compex. Corr. Factor
1.1.2.10	"	Conc. of SO_4 Aq. at Bottom of Unsat. Zone from Pyrite
1.1.2.11	"	Conc. of SO_4 Aq. Bottom Unsat. Zone
1.1.2.12	"	Conc. Uncomp. SO_4 Bottom Unsat. Zone
1.1.2.13	"	Conc. of SO_4 Aq. in Mixing Layer from Pyrite
1.1.3.1	"	Conc. of SO_4 Aq. at Gypsum-Depleted Front
1.1.3.2	"	pH Layer 1
1.1.4	Calculate	pH Layer 3
1.1.4.1	"	Hyp. SO_4 in Mixing Layer no Gyp.
1.1.4.2	"	Fe(III) Bottom Unsat. Zone
1.1.4.3	"	Conc. Fe(II) in Mixing Layer
1.1.4.4	"	Conc. of SO_4 Aq. in Mixing Layer
1.1.4.5	"	Gyp. Diss. in Mixing Zone
1.1.4.6	"	Conc. of SO_4 Aq. in Mixing Layer
1.1.4.7	"	Conc. of Ca Aq. in Mixing Layer
1.1.4.8	"	pH Layer 3
1.1.5	Calculate	pH Layer 4
1.1.5.1	"	Conc. of SO_4 Aq. in Bottom Layer from Pyrite
1.1.5.2	"	Conc. Fe(II) in Bottom Layer
1.1.5.3	"	Conc. of SO_4 Aq. in Bottom Layer
1.1.5.4	"	Conc. of Ca Aq. in Bottom Layer
1.1.5.5	"	pH Layer 4
1.2	Calculate	Uranium Source Concentrations
1.2.1	"	Init. Conc. U in Tailings Solid
1.2.2	"	Mole Fract. U_3O_8 in Pyrite
1.2.3	"	Conc. Solid U in Unsat. Zone
1.2.4	"	Aq. U in Unsat. Zone
1.2.5	"	Aq. U in Mixing Zone
1.2.6	"	Aq. U in Bottom Layer
1.3	Calculate	Thorium Source Concentrations
1.3.1	"	Time Independent Th Parameters
1.3.1.1	"	Init. Activ. Th-230 in Tailings
1.3.1.2	"	Init. Conc. Solu. Th-232
1.3.1.3	"	Init. Conc. Insolu. Th-232
1.3.1.4	"	Init. Solid Phase Conc. of Th-230
1.3.1.5	"	Init. Conc. Solu. Th-230
1.3.1.6	"	Init. Conc. Insolu. Th-230
1.3.1.7A	"	Activ. Fract. Th-232 in Solu. Th
1.3.1.7B	"	Activ. Fract. Th-230 in Solu. Th
1.3.1.8	"	Init. Conc. Total Solu. Th
1.3.1.9	"	Mole Fract. Th-230
1.3.1.10	"	Mole Fract. Th-232
1.3.1.11	"	Wt. Th Convers. Factor
1.3.1.12	"	Log Appar. Solu. Prod. $Th(OH)_4$
1.3.2	Calculate	Time Dependent Thorium Parameters
1.3.2.1A	"	Aq. Th in Unsat. Zone
1.3.2.1B	"	Conc. Total Th Diss.

Table B1 cont'd

1.3.2.2	Calculate Conc. Diss. Th-232 in Unsat. Zone
1.3.2.3	" Conc. Solid Th-230 in Unsat. Zone
1.3.2.4	Recalculate Aq. Th in Unsat. Zone
1.3.2.5A	Calculate Conc. Diss. Th-232 in Unsat. Zone
1.3.2.5B	" Total Th in Solid Phase Unsat. Zone
1.3.2.5C	Calculate Activ. Fract. Th-232 in Surf. Solid Th
1.3.2.6A	" Aq. Th in Mixing Layer
1.3.2.6B	" Conc. Total Th Diss. in Mixing Layer
1.3.2.7	Recalculate Aq. Th in Mixing Layer
1.3.2.8	Calculate Aq. Th in Bottom Sat. Zone
1.4	Calculate Radium Source Concentrations
1.4.1	" Conc. Solid Ra in Layer 1
1.4.1.1	" Ingrowth Factor for Ra-226
1.4.1.2	" Init. Solid Phase Conc. Ra-226 in Tailings
1.4.1.3	" Cum. Solid Conc. Ra-226 from Th-230
1.4.1.4	" Conc. Solid Ra in Layer 1
1.4.2	Calculate Barium Concentrations
1.4.2.1	" Sq. Root Eqbm. Const. $BaSO_4$
1.4.2.2	" Init. Solid Conc. $BaSO_4$
1.4.2.3	" Incr. $BaSO_4$ Depleted Layer
1.4.2.4	" Thickness $BaSO_4$ Depleted Layer
1.4.2.5	" Total Ba Conc. Bottom Unsat. Zone
1.4.2.6	" Reprecip. $BaSO_4$
1.4.3	Calculate Radium Concentrations in Layer 2
1.4.3.1	" Mole Fract. Ra-226
1.4.3.2	" Conc. Ra-226 from Ingrowth in Δt, Unsat.
1.4.3.3	" Mole Fract. Ra-226 in $BaSO_4$ Solid
1.4.3.4	" Conc. Solid Ra in Layer 2
1.4.3.5	" Aq. Ra Bottom Unsat. Zone
1.4.4	Calculate Radium Concentrations in Sat. Zone
1.4.4.1	" Ra Assoc. Ba Unsat. Plus Mix
1.4.4.2	" Conc. Ra-226 from Ingrowth in Δt, Mixing
1.4.4.3	" Conc. Ra Mixing Zone Inputs
1.4.4.4A	" Sum Dissolved Ra
1.4.4.4B	Recalculate Conc. Ra Mixing Zone Inputs
1.4.4.5	Calculate Aq. Ra in Mixing Zone
1.4.4.6	" Conc. Ra-226 from Ingrowth in Δt, Bottom
1.4.4.7	" Conc. Ra Bottom Zone Inputs
1.4.4.8	" Aq. Ra in Bottom Sat. Zone
1.5	Calculate Pb-210 Source Concentrations
1.5.1	" Conc. Solid Pb-210 in Layer 1
1.5.1.1	" Ingrowth for Pb-210
1.5.1.2	" Init. Solid Phase Conc. Pb-210 in Tailings
1.5.1.3	" Conc. Solid Pb-210 in Layer 1
1.5.2	Calculate Aq. Conc. Pb-210 at the Bottom of the Unsaturated Zone
1.5.2.1	Calculate Sq. Root Eqbm. Const. $PbSO_4$
1.5.2.2	" Total Aq. Pb Conc. Bottom Unsat. Zone
1.5.2.3	" Mole Fract. Pb-210
1.5.2.4	" Conc. Pb-210 from Ingrowth in Δt, Unsat.
1.5.2.5	" Incr. $PbSO_4$ Depleted Layer

Table B1 cont'd

1.5.2.6	Calculate	Thickness $PbSO_4$ Depleted Layer
1.5.2.7	"	Aq. Pb-210 Bottom Unsat. Zone
1.5.3	Calculate	Pb-210 Concentrations in Saturated Zone
1.5.3.1	"	Pb-210 Assoc. $PbSO_4$, Unsat. Plus Mix
1.5.3.2	"	Conc. Pb-210 from Ingrowth in Δt, Mixing
1.5.3.3	"	Conc. Pb-210 Mixing Zone Inputs
1.5.3.4A	"	Sum Dissolved Pb-210
1.5.3.4B	Recalculate	Conc. Pb-210 Mixing Zone Inputs
1.5.3.5	Calculate	Aq. Pb-210 Mixing Layer
1.5.3.6	"	Conc. Pb-210 from Ingrowth in Δt, Bottom
1.5.3.7	"	Conc. Pb-210 Bottom Layer Inputs
1.5.3.8	"	Aq. Pb-210 Bottom Unsat. Zone
1.6	Calculate	Mass Loss from Tailings by Erosion
1.6.1	"	Bedload Transport Capacity
1.6.1.1	"	Total Length of Tailings Pile
1.6.1.2	"	Number of Slope Elements
1.6.1.3	"	Length of a Slope Element
1.6.1.4	"	Median Particle Size
1.6.1.5	"	Transport Soil (Bedload)
1.6.1.6	"	Exponent in Bedload Eqn
1.6.1.7	"	Fract. Tailings Veg.
1.6.1.8	"	Runoff Reduction Factor
1.6.1.9	"	Transport Redn. Factor
1.6.1.10	"	Total Length to End Segment "eseg"
1.6.1.11	"	Bedload Transport Capacity
1.6.2	Calculate	Fraction of Sediment Trapped
1.6.2.1	"	Average Grass Spacing
1.6.2.2	"	Flow Velocity Through Grass
1.6.2.3	"	Depth of Flow
1.6.2.4	"	Spacing Hydraulic Radium
1.6.2.5	"	Mean Silt Diameter
1.6.2.6	"	Settling Velocity
1.6.2.7	"	Fract. Trapped Sed.
1.6.3	Calculate	Mass Loss from Tailings by Erosion
1.6.3.1	"	Exposed Tailings Surface Area
1.6.3.2	"	Control Practice Factor
1.6.3.3	"	Segment Slope Factor
1.6.3.4	"	Soil Erodibility Factor
1.6.3.5	"	Sediment Detached in Segment "eseg"
1.6.3.6	"	Sediment Available for Transport
1.6.3.7	"	Bedload for Segment
1.6.3.8	Deleted	
1.6.3.9	Deleted	
1.6.3.10	Calculate	Erosion Mass Loss from Tailings
2.0	Calculate	Concentrations from Atmospheric Pathways
2.1	"	Ann. Avg. Emission Rate U, Th, Ra, Pb in Dust from Tailings
2.2	Calculate	Ann. Avg. Emission Rate of Rn Gas from Tailings
2.2.1	"	Ann. Avg. Emission Rate of Rn Gas from Tailings

Table B1 cont'd

2.2.2	Calculate	Rn Flux from the Entire Unsaturated Zone
2.2.3	"	Rn Activity Emanating from the Upper (Lower) Unsat. Zone
2.2.4	"	the Reciprocal of Rn Diffusion Path Length
2.3	Calculate	Conc. of Contaminants in Air at 80 Receptor Locations and Study Area and Watershed Average Conc.
2.3.1	Calculate	Fraction of Time Wind Blows to Receptor
2.3.2	"	Mean Wind Speed, Source to Receptor
2.3.3	"	Effective Distance from Source to Receptor
2.3.4	"	Vertical Dispersion Coefficient
2.3.5	"	Conc. of Contaminant in Air at Receptor
2.3.6	"	Conc. of Contaminant in Air, Watershed Avg.
2.3.7	"	Conc. of Contaminant in Air, Study Area Avg.
2.3.7A	Calculate	Ring Areas
2.4	Calculate	Radionuclide Conc. in Soil Layers
2.4.1	"	Radionuclide Input for Soil Layer 1
2.4.2	"	Leaching Loss Rate Constant
2.4.3	"	Radionuclide Activity Soil Layer 1
2.4.4	"	Avg. Aq. Radionuclide Conc. in Soil Layer
2.4.5	"	Radionuclide Activity Soil Layer (sla>2)
2.4.6	"	Radionuclide Conc. in Soil Layer
2.5	Calculate	Total Groundshine Dose Rate
2.5.1	"	Total Gamma Rays, Ra-226 Chain
2.5.2	"	Avg. Energy for Ra-226 Chain in Energy Band
2.5.3	"	Linear Attenuation Coefficient for Soil Layer
2.5.4	"	Flux from a Soil Layer
2.5.5	"	Total Soil Surface Flux
2.5.6	"	Total Groundshine Dose Rate for Radionuclide Chain
2.5.7	"	Total External Dose Rate from Groundshine
2.6	Calculate	Conc. of Radionuclide in Vegetation
3.0	Calculate	Watershed Aqueous Solution Radionuclide Concentration
3.1	"	Groundwater Radionuclide Discharge Conc.
3.1.1	"	Retardation Factor
3.1.2	"	Volumetric Seepage
3.1.3	"	Darcy Velocity
3.1.4	"	Longitudinal Dispersion Coefficient
3.1.5	"	Green's Function
3.1.6	"	Discharge Concentration Not Including Ingrowth
3.1.7	"	Groundwater Radionuclide Discharge Conc.
3.2	Calculate	pH of Lake n
3.2.1	"	Source Term Volume Discharge
3.2.2	"	Volume of Lake n
3.2.3	"	Flow

Table B1 cont'd

3.2.4	Calculate	Retention Time in Lake n
3.2.5	"	Ca Conc. at Node 1
3.2.5A	"	SO_4 Conc. at Node 1
3.2.6	"	Ca (and SO_4) Conc. at Node n (n>1)
3.2.7	"	pH of Lake
3.3	Calculate	Watershed Aqueous Solution Radionuclide Concentrations
3.3.1	"	Lake K_d for Th
3.3.2	"	Mass Transfer Coefficient, Lake
3.3.3	"	Rate Const. Removal to Sediment
3.3.4	"	Rate Const. for Release from Sediment
3.3.5	"	Rate Const. for Radionuclide Burial
3.3.6	"	Calculate Conc. of Radionuclide in Water at Node 1
3.3.7	"	Radionuclide Decay Factor
3.3.8	"	Calculate Quantity Radionuclide in Solution in Lakes
3.3.8.1	"	Matrix Parameters Used in WATEX
3.3.8.2	"	KS Parameter Used in WATEX
3.3.8.3	"	KW Parameter Used in WATEX
3.3.8.4	"	V1 Parameter Used in WATEX
3.3.8.5	"	V2 Parameter Used in WATEX
3.3.8.6	"	X Parameter Used in WATEX
3.3.8.7	"	Y Parameter Used in WATEX
3.3.8.8	"	AA Parameter Used in WATEX
3.3.8.9	"	BB Parameter Used in WATEX
3.3.8.10	"	Quantity of Radionuclides in Lake Water Col.
3.3.8.11	"	Quantity of Radionuclides in Lake Sediment Exch. Zone
3.3.9	Calculate	Conc. of Radionuclide in Water at Watershed Node n
4.0	Calculate	Dose
4.1	"	Ingestion Doses
4.1.1	"	Ingest. of Veg. Dose
4.1.2	"	Ingest. of Moose Dose
4.1.2.1	"	Avg. Conc. in Watershed
4.1.2.2	"	Conc. in Moose Aquatic Foods
4.1.2.3	"	Water-Moose Conc.
4.1.2.4	"	Air-Moose Conc.
4.1.2.5	"	Moose Dose
4.1.3	Calculate	Ingest. of Caribou Dose
4.1.3.1	"	Air-Caribou Conc.
4.1.3.2	"	Water-Caribou Conc.
4.1.3.3	"	Caribou Dose
4.1.4	Calculate	Ingest. of D.W. Dose
4.1.5	Calculate	Ingestion of Fish Dose
4.1.5.1	"	Fish Availability
4.1.5.2	"	Fish Conc.
4.1.5.3	"	Ingest. of Fish Dose

Table B1 concluded

4.2	Calculate	Inhalation Doses
4.2.1	"	Dust Dose
4.2.2	"	Rn Gas dose
4.3	Calculate	Internal Doses
4.4	Calculate	Total Internal Dose

Table B2 Cross-Reference for Variables and Their DDDs

Variable name	DDD number
A11, A21, etc.	3.3.8.1
AA(nuc,n)	3.3.8.8
ACARC(nuc)	4.1.3.1
AEXPT	1.6.3.1
AIRC(nuc,loc)	2.3.5,.6,.7
AIRDIS	3.1.4
AMOC(nuc)	4.1.2.4
APBI	1.5.1.2
AQVEGC(nuc)	4.1.2.2
ARADI	1.4.1.2
AT230I	1.3.1.1
AU238O	1.3.1.1
AUNATO	1.2.1
AUNATT	1.2.1
AVEGC(nuc,loc)	2.6
BASATI	1.4.4.1
BB(nuc,n)	3.3.8.9
BED(eseg)	1.6.3.7
BETA	1.1.2.4
BETAO(nuc,sla,loc)	2.4.1,.5
BETAI(nuc,sla,loc)	2.4.2
BEXP	1.6.1.6
BGW(nuc)	3.1.5
BRWSC(nuc)	2.6
BVEGC(nuc)	2.6
CALIME	1.1.2.7
CARDOS(nuc)	4.1.3.3
CBAR	1.4.2.5
CBARI	1.4.2.2
CIGPB	3.1.7
CLEAD	1.5.2.2
CONC(1,1,1)	1.2.1
CONC(1,1,3)	1.2.3
CONC(2,1,3)	1.3.2.5B
CONC(3,1,3)	1.5.1.3
CONC(4,1,3)	1.4.1.4
CONC(4,2,3)	1.4.3.4
CPBI	1.5.1.2
CPBIN3	1.5.3.3,.4B
CPBIN4	1.5.3.7

Table B2 cont'd

CPBRAS	1.5.1.3
CPBRL2	1.5.2.4
CPBRL3	1.5.3.2
CPBRL4	1.5.3.6
CPBTI	1.5.1.3
CRADI	1.4.1.2
CRADTI	1.4.1.4
CRAIN3	1.4.4.3,.4B
CRAIN4	1.4.4.7
CRATHS	1.4.1.3
CRATL2	1.4.3.2
CRATL3	1.4.4.2
CRATL4	1.4.4.6
CRO	1.6.1.8
CSOIL	1.6.3.2
CT230I	1.3.1.4
CT232I	1.3.1.2
CTSOIL	1.6.1.9
CVEG(nuc,v,loc)	2.6
D50	1.6.1.4
DBAR	1.4.2.4
DBOT	1.1.1.4
DCFHA(Th)	4.2.1
DCFGA(Th)	4.1.2.5
DCFWAT(Th)	4.1.2.5
DELT	1.1.2.9
DELTAG	1.1.4.5
DELTAH	1.1.2.6
DETIME(n)	3.2.4
DF	1.6.2.3
DFR(nuc)	3.3.7
DGYP	1.1.2.6
DHBAR	1.4.2.3
DHLEAD	1.5.2.5
DIFLEN	2.2.4
DLEAD	1.5.2.6
DMID	1.6.2.5
DOSEGS(loc)	2.5.7
DOSEIA	4.4
DOSEIC	4.4
DRYRHO	2.6
DUSDIA	4.3
DUSDIC	4.3
DV	3.1.3
EBKDFC	2.2.4

Table B2 cont'd

EMRATE(nuc)	2.1
EMRATE(RN)	2.2.1
ENERGY(Ra,band)	2.5.2
EQUIL	1.1.1.2
EQUILB	1.4.2.1
EQUILP	1.5.2.1
EROTOT	1.6.3.10
ESOIL	1.6.3.5
FAIAM	4.1.2.3
FISHA(n)	4.1.5.1
FISHC(nuc,n)	4.1.5.2
FISHD(nuc,n)	4.1.5.3
FLOWQ(n)	3.2.3
FLXSL(nuc,band,sla,loc)	2.5.4
FLXTOT(nuc,band,loc)	2.5.5
FNG(nuc)	3.1.5
FSHDIA	4.3
FSHDIC	4.3
FT	4.1.3.2
FVEG	1.6.1.7
FWINDT	2.1
FWIND1	2.3.5
FWIND2(dir,st)	2.3.1
GDOS(nuc,band,loc)	2.5.6
GDOSN(nuc,loc)	2.5.6
GWATC(nuc)	3.1.7
GWATP(nuc)	3.1.6
GYPI	1.1.1.1
GYPM1X	1.1.4.5
IGPB	1.5.1.1
IGRA	1.4.1.1
INHD(nuc,loc)	4.2.1
INLIME	1.1.2.5
K1(nuc,n)	3.3.3
K2(nuc,n)	3.3.4
K3(nuc,n)	3.3.5
KRATE	1.1.2.3
KS(nuc,n)	3.3.8.2
KSOIL	1.6.3.4
KW(nuc,n)	3.3.8.2
LAKVOL(n)	3.2.2
LDC	3.1.4
LENGT	1.6.1.1
LENGTH	1.6.1.3
LENTOT(eseg)	1.6.1.10

Table B2 cont'd

LICHC(nuc)	2.6
LIMEIN	1.1.1.3
MBAR	1.4.2.6
METDIA	4.3
METDIC	4.3
MODOS(nuc)	4.1.2.5
MSLP	1.6.3.5
MSOIL	1.6.3.4
MU(nuc,band,sla)	2.5.3
MUD(nuc,band,sla)	2.5.4
NDEC(Ra,band)	2.5.1
NLEN	1.6.1.2
PBSTI	1.5.3.1
PH1	1.1.3.2
PH2	1.1.2.8
PH3	1.1.4.8
PH4	1.1.5.5
PYRITE	1.1.2.1
Q(nuc)	2.1
R(nuc)	3.1.1
RADD(loc)	4.2.2
RAREA	2.3.7a
RNDIA	4.3
RNDIC	4.3
RNFLUX	2.2.2
RNFXAV	2.2.1
RNGMDA(dis)	2.3.3
RS	1.6.2.4
RTCCA(n)	3.2.6
RTCS(n)	3.2.6
SIP	2.2.3
S2P	2.2.3
SFLOW	3.2.1
SFLUX	1.1.2.2
SLPFAC	1.6.3.3
SOILC(nuc,loc)	2.6
SOILCN(nuc,sla,loc)	2.4.6
SPACE	1.6.2.1
SSTAR	1.1.4.1
SUFOC(nuc)	2.6
SUMBAR	1.4.4.4A
SUMPB	1.5.3.4A
SUNCOM	1.1.2.12
SUS(eseg)	1.6.3.6
SWCONC(nuc,sla)	2.4.4
T230D	1.3.2.3

Table B2 cont'd

T230IS	1.3.1.6
T230S	1.3.2.3
T230SO	1.3.1.5
T232D	1.3.2.2
T232IS	1.3.1.3
T232S	1.3.2.5A
T232SO	1.3.1.2
TAREA	2.3.7A
TCSOIL(eseg)	1.6.1.11
THDISM	1.3.2.6B
THDISS	1.3.2.1B
THORCF	1.3.1.11
THORDC	1.3.1.12
THSOL	1.3.1.8
TRSED	1.6.2.7
TSOIL	1.6.1.5
TVEG	1.6.1.7
UPYRI	1.2.2
UWIND(dir,st)	2.3.2
V1(nuc,n)	3.3.8.4
V2(nuc,n)	3.3.8.5
VDISP(dis,st)	2.3.4
VEGD(nuc,loc)	4.1.1
VEGDIA	4.3
VEGDIC	4.3
VEL	1.6.2.2
VELRAT	1.6.1.9
VS	1.6.2.6
VSR	3.1.2
WATAVG(nuc)	4.1.2.1
WATC(nuc,n)	3.3.6,.9
WATCCA(n)	3.2.5,.6
WATCS(n)	3.2.5A,.6
WATD(nuc,loc)	4.1.4
WATDIA	4.3
WATDIC	4.3
WATKL(n)	3.3.2
WATPH(n)	3.2.7
WATRS(nuc,n)	3.3.8.11
WATRW(nuc,n)	3.3.8.10
WCARC(nuc)	4.1.3.2
WCONC(1,2,3)	1.2.4
WCONC(1,3,3)	1.2.5
WCONC(1,4,3)	1.2.6
WCONC(2,2,3)	1.3.2.1A,.4

Table B2 cont'd

WCONC(2,3,3)	1.3.2.6A,.7
WCONC(2,4,3)	1.3.2.8
WCONC(3,2,3)	1.5.2.7
WCONC(3,3,3)	1.5.3.5
WCONC(3,4,3)	1.5.3.8
WCONC(4,2,3)	1.4.3.5
WCONC(4,3,3)	1.4.4.5
WCONC(4,4,3)	1.4.4.8
WCONC(6,2,3)	1.1.2.10
WCONC(6,3,3)	1.1.2.13
WCONC(6,4,3)	1.1.5.1
WCONC(7,1,3)	1.1.3.1
WCONC(7,2,3)	1.1.2.11
WCONC(7,3,3)	1.1.4.4/.6
WCONC(7,4,3)	1.1.5.3
WCONC(8,2,3)	1.1.2.8
WCONC(8,3,3)	1.1.4.7
WCONC(8,4,3)	1.1.5.4
WCONC(9,2,3)	1.1.4.2
WCONC(10,3,3)	1.1.4.3
WCONC(10,4,3)	1.1.5.2
WKDTH(n)	3.3.1
WMOC(nuc)	4.1.2.3
WSIGD(n)	3.3.5
X(nuc,n)	3.3.8.6
X230LA	1.3.1.7B
X230LM	1.3.1.9
X232LA	1.3.1.7A
X232LM	1.3.1.10
X232SA	1.3.2.5C
XBAR	1.4.3.3
XLEAD	1.5.2.3
XPBI	1.5.2.3
XRAD	1.4.3.1
XURANI	1.2.2
Y(nuc,n)	3.3.8.7
ZAVG(nuc)	2.4.4
ZTOT(nuc,sla,loc)	2.4.3,.5

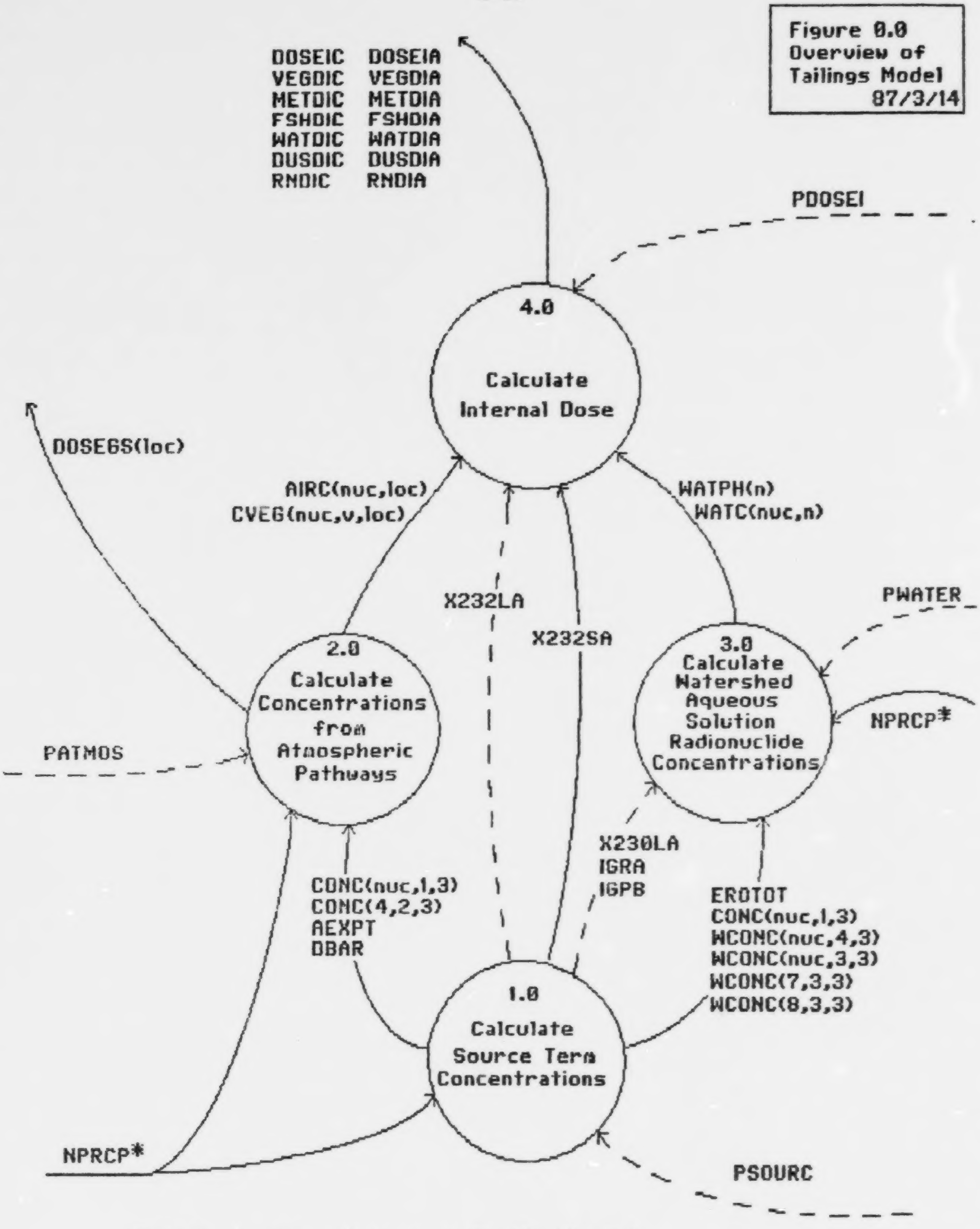
DOSEIC DOSEIA
VEGDIC VEGDIA
METDIC METDIA
FSHDIC FSHDIA
WATDIC WATDIA
DUSDIC DUSDIA
RNDIC RNDIA
PDOSEI
4.0
Calculate Internal Dose
DOSEGS(loc)
AIRC(nuc,loc)
CVEG(nuc,v,loc)
WATPH(n)
WATC(nuc,n)
X232LA
X232SA
PWATER
2.0
Calculate Concentrations from Atmospheric Pathways
3.0
Calculate Watershed Aqueous Solution Radionuclide Concentrations
NPRCP*
PATMOS
X230LA
IGRA
IGPB
CONC(nuc,1,3)
CONC(4,2,3)
AEXPT
DBAR
EROTOT
CONC(nuc,1,3)
WCONC(nuc,4,3)
WCONC(nuc,3,3)
WCONC(7,3,3)
WCONC(8,3,3)
1.0
Calculate Source Term Concentrations
NPRCP*
PSOURC

Figure 0.0
Overview of
Tailings Model
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Notes:
1. nuc = 1, 2, 3, 4 (U, Th, Pb, Ra).
   For AIRC, nuc = 5 is for Rn.
2. v = 1 to 5 (vegetation classes).
3. loc = 1 to 82 (locations, including two 'average' locations).
4. n = 1 to 8 (watershed nodes).

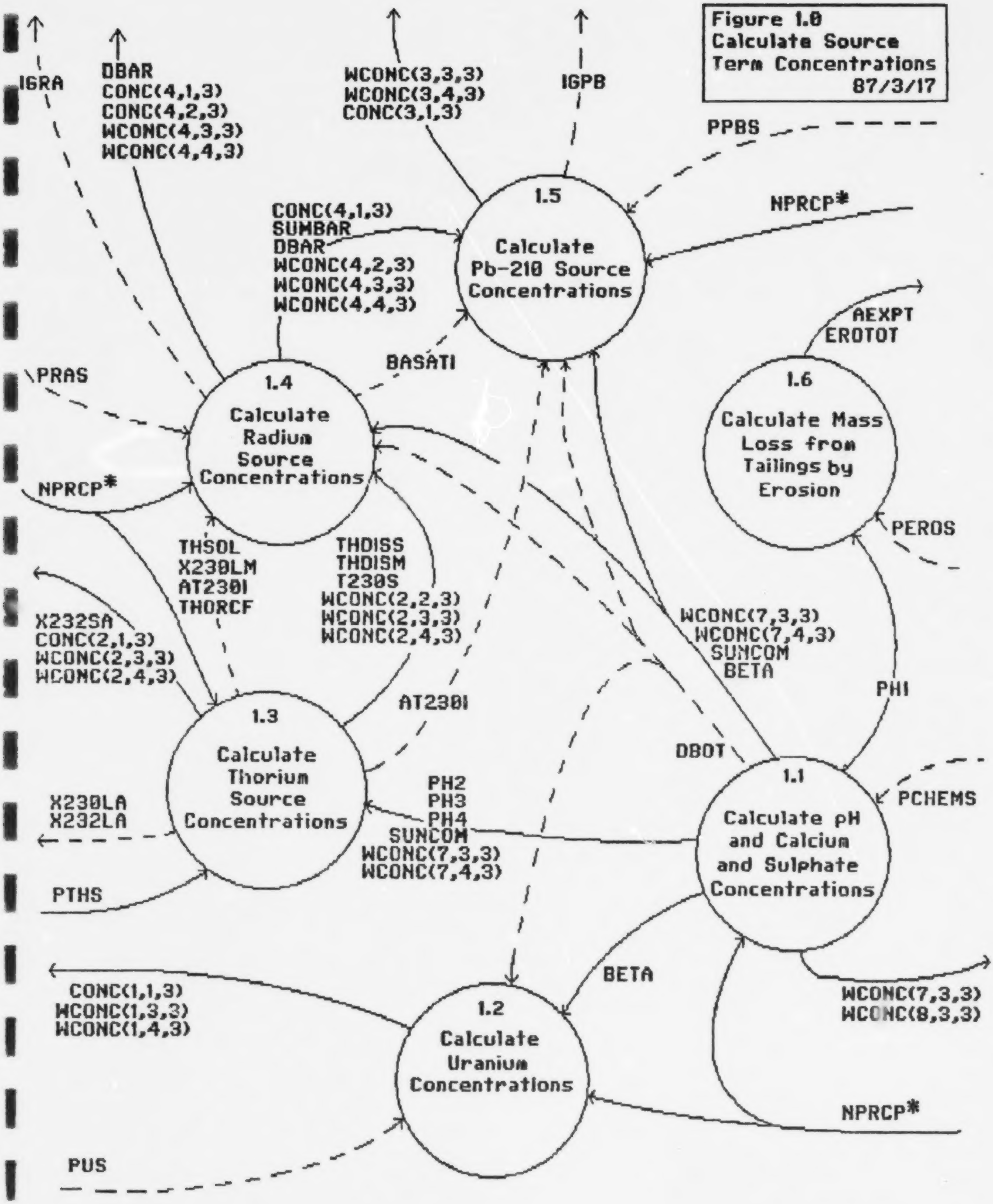


Figure 1.0
Calculate Source
Term Concentrations
87/3/17

IGRA
DBAR
CONC(4,1,3)
CONC(4,2,3)
WCONC(4,3,3)
WCONC(4,4,3)
WCONC(3,3,3)
WCONC(3,4,3)
CONC(3,1,3)
IGPB
PPBS
1.5
Calculate
Pb-210 Source
Concentrations
NPRCP*
CONC(4,1,3)
SUMBAR
DBAR
WCONC(4,2,3)
WCONC(4,3,3)
WCONC(4,4,3)
BASATI
AEXPT
EROTOT
PRAS
1.4
Calculate
Radium
Source
Concentrations
NPRCP*
1.6
Calculate Mass
Loss from
Tailings by
Erosion
PEROS
THSOL
X230LM
AT230I
THORCF
THDISS
THDISM
T230S
WCONC(2,2,3)
WCONC(2,3,3)
WCONC(2,4,3)
X232SA
CONC(2,1,3)
WCONC(2,3,3)
WCONC(2,4,3)
WCONC(7,3,3)
WCONC(7,4,3)
SUNCOM
BETA
PHI
AT230I
1.3
Calculate
Thorium
Source
Concentrations
DBOT
1.1
Calculate pH
and Calcium
and Sulphate
Concentrations
PCHEMS
X230LA
X232LA
PH2
PH3
PH4
SUNCOM
WCONC(7,3,3)
WCONC(7,4,3)
PTHS
BETA
WCONC(7,3,3)
WCONC(8,3,3)
CONC(1,1,3)
WCONC(1,3,3)
WCONC(1,4,3)
1.2
Calculate
Uranium
Concentrations
NPRCP*
PUS

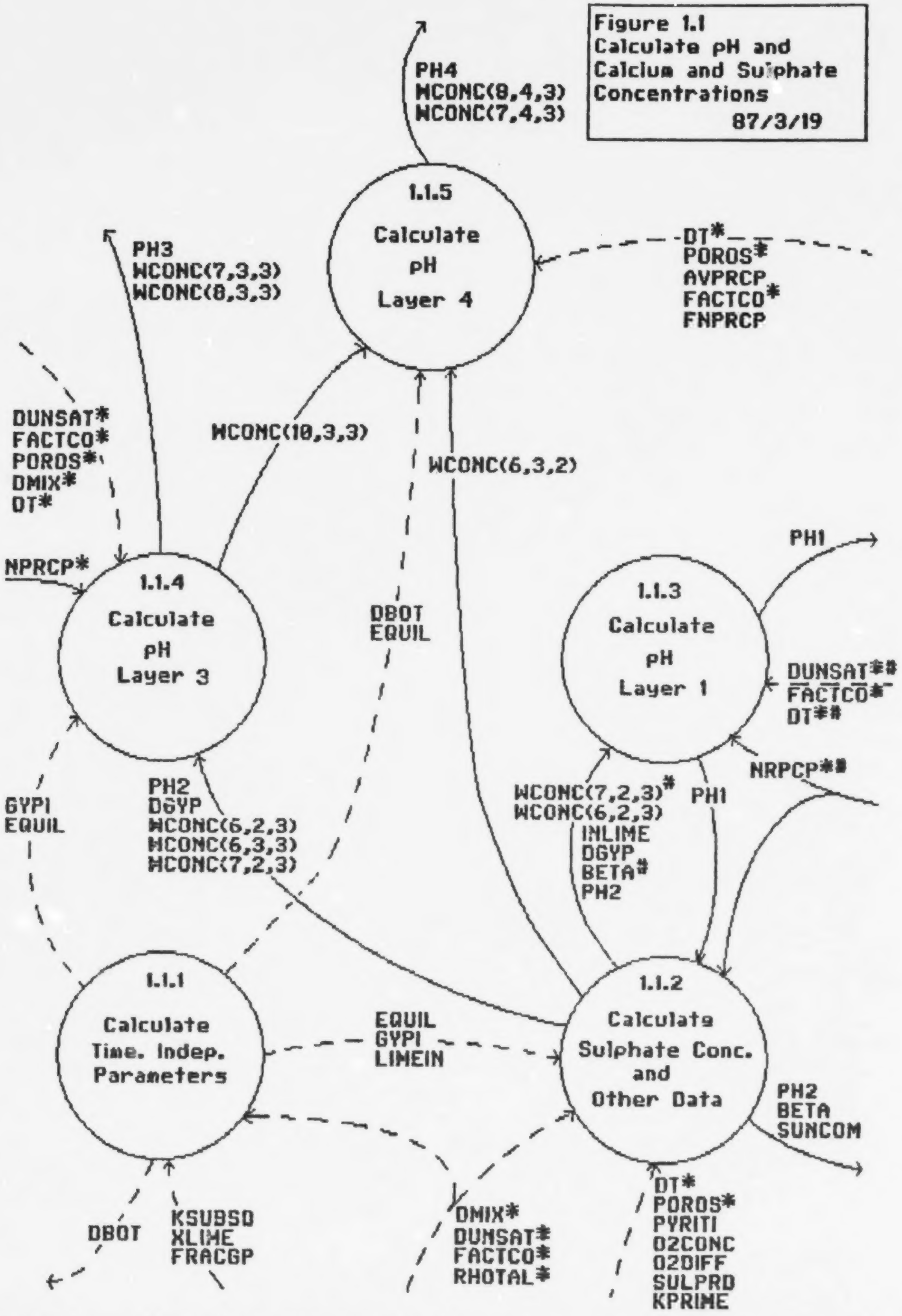
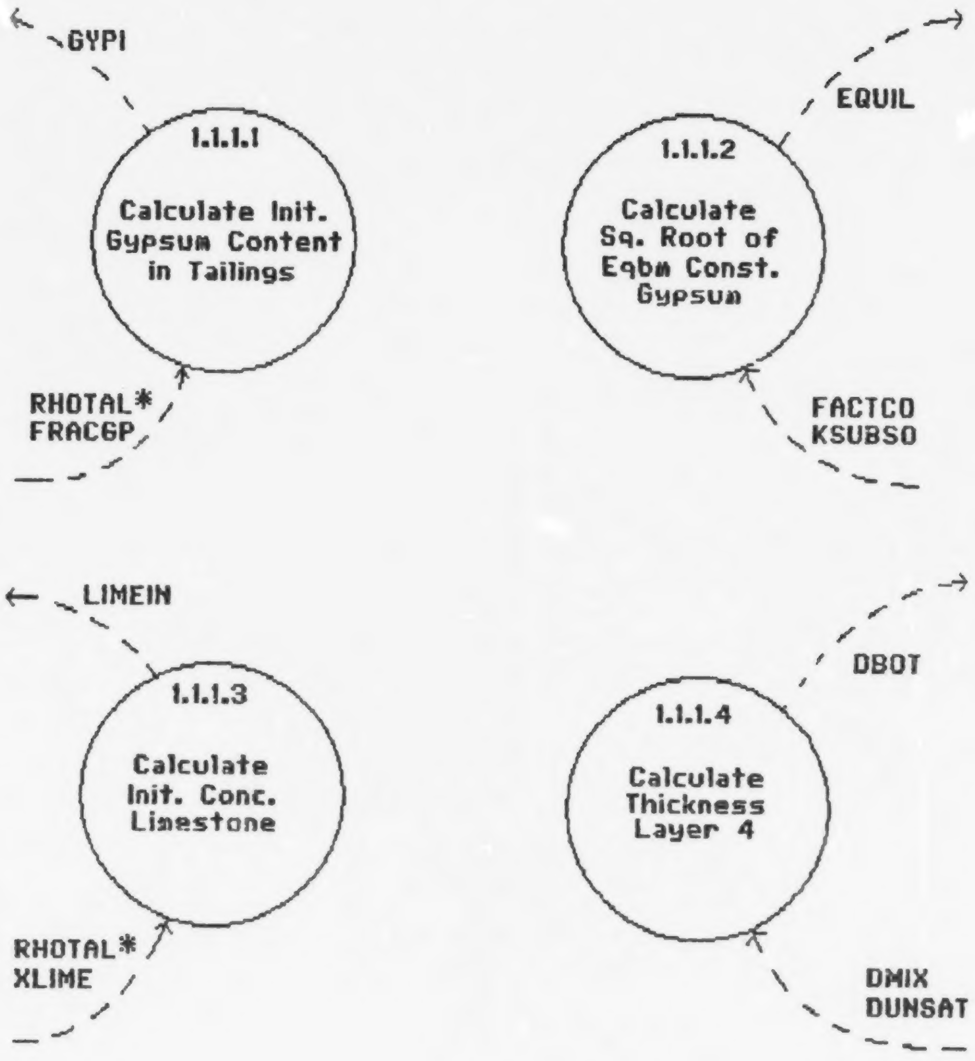


Figure 1.1
Calculate pH and
Calcium and Sulphate
Concentrations
87/3/19

PH4
WCONC(8,4,3)
WCONC(7,4,3)
1.1.5
Calculate
pH
Layer 4
DT*
POROS*
AVPRCP
FACTCO*
FNPRCP
PH3
WCONC(7,3,3)
WCONC(8,3,3)
DUNSAT*
FACTCO*
POROS*
DMIX*
DT*
WCONC(10,3,3)
WCONC(6,3,2)
NPRCP*
1.1.4
Calculate
pH
Layer 3
DBOT
EQUIL
PH1
1.1.3
Calculate
pH
Layer 1
DUNSAT*#
FACTCO*
DT*#
NRPCP*#
GYPI
EQUIL
PH2
DGYP
WCONC(6,2,3)
WCONC(6,3,3)
WCONC(7,2,3)
WCONC(7,2,3)*
WCONC(6,2,3)
INLIME
DGYP
BETA#
PH2
PH1
1.1.1
Calculate
Time. Indep.
Parameters
EQUIL
GYPI
LIMEIN
1.1.2
Calculate
Sulphate Conc.
and
Other Data
PH2
BETA
SUNCOM
DBOT
KSUBSO
XLIME
FRACGP
DMIX*
DUNSAT*
FACTCO*
RHOTAL*
DT*
POROS*
PYRITI
O2CONC
O2DIFF
SULPRD
KPRIME

Note: inspection of the UTAP2 code shows that the parameters marked with a "#" are not required in the DFD.

Figure 1.1.1
Calculate Time
Indep. Parameters
87/3/19


GYPI
1.1.1.1
Calculate Init. Gypsum Content in Tailings
RHOTAL*
FRACGP
EQUIL
1.1.1.2
Calculate Sq. Root of Eqbm Const. Gypsum
FACTCO
KSUBSO
LIMEIN
1.1.1.3
Calculate Init. Conc. Limestone
RHOTAL*
XLIME
DBOT
1.1.1.4
Calculate Thickness Layer 4
DMIX
DUNSAT

GYPI - INIT. GYPSUM CONTENT IN TAILINGS [mol m^{-3}].
Initial gypsum content of tailings.

Figure 1.1.1.1
Calculate INIT. GYPSUM
CONTENT IN TAILINGS
(GYPI)

FRACGP
RHOTAL - - -> GYPI

Short Name	Long Name	SI Unit	Source
FRACGP	MASS FRAC. OF GYPSUM IN TAILINGS	[-]	Sampled
GYPI	INIT. GYPSUM CONTENT IN TAILINGS	[mol m^{-3}]	1.1.1.1
RHOTAL	TAILINGS BULK DENSITY	[g m^{-3}]	Sampled

$$GYPI = \frac{RHOTAL * FRACGP}{136} \qquad \text{(eqn. 3.2.2)}$$

Unit check: $[g\ m^{-3}] * [-] / [g\ mol^{-1}] = [mol\ m^{-3}]$

Note 1: The constant (136) has units of [g mol^{-1}] and corresponds to the molecular weight of anhydrous $CaSO_4$ (SENES Vol. 3, pg 3.3).

Figure 1.1.1.2
Calculate SQ. ROOT OF EQBM. CONST. GYPSUM (EQUIL)

EQUIL - SQ. ROOT OF EQBM. CONST. GYPSUM [mol m^{-3}]. EQUIL is an intermediate parameter, equal to the square root of the solubility product for gypsum, divided by the activity coefficient.

KSUBSO
FACTCO - - -> EQUIL

Short Name	Long Name	SI Unit	Source
EQUIL	SQ. ROOT OF EQBM. CONST. GYPSUM	[mol m^{-3}]	1.1.1.2
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
KSUBSO	SOLUBILITY EQBM. CONST. FOR GYPSUM	[mol^2 m^{-6}]	Sampled

$$\mathrm{EQUIL} = \frac{\mathrm{KSUBSO}^{1/2}}{\mathrm{FACTCO}}$$ (eqn. near eqn. 3.3.22)

Unit check: $[\mathrm{mol}^2\ \mathrm{m}^{-6}]^{1/2}\ /\ [-]\ =\ [\mathrm{mol}\ \mathrm{m}^{-3}]$

Note: $K^\circ_s = K^\circ_{s,CaSO_4}$ has been assumed.

Figure 1.1.1.3
Calculate
INIT. CONC. LIMESTONE
(LIMEIN)

LIMEIN - INIT. CONC. LIMESTONE [mol m^{-3}]. Initial concentration of limestone (as $CaCO_3$) in the tailings.

$$\left.\begin{array}{l}\text{XLIME}\\ \text{RHOTAL}\end{array}\right. \;\text{- - ->}\; \text{LIMEIN}$$

Short Name	Long Name	SI Unit	Source
LIMEIN	INIT. CONC. LIMESTONE	[mol m^{-3}]	1.1.1.3
RHOTAL	TAILINGS BULK DENSITY	[g m^{-3}]	Sampled
XLIME	INIT. MASS FRACT. LIME	[-]	Sampled

$$\text{LIMEIN} = \text{XLIME} * \text{RHOTAL} / 100 \qquad \text{(eqn. 3.3.45)}$$

Unit check:

$$\frac{[-] * [\text{g m}^{-3}]}{[\text{g mol}^{-1}]} = [\text{mol m}^{-3}]$$

Note 1: 100 is the mass of one mole of $CaCO_3$ [g mol^{-1}].

Note 2: The value of XLIME determines the scenario. If no limestone has been added to the tailings XLIME = 0.0. If limestone has been added, the only case considered is when XLIME = 0.01 (i.e., the limestone is 1% the total tailings mass). See SENES Vol. 3, section 2.7.

DBOT - THICKNESS LAYER 4 [m]. The thickness of the bottom layer of the tailings (layer 4) below the mixing zone.

Figure 1.1.1.4
Calculate
THICKNESS LAYER 4
(DBOT)

DUNSAT
DMIX --> DBOT

Short Name	Long Name	SI Unit	Source
DBOT	THICKNESS LAYER 4	[m]	1.1.1.4
DMIX	THICKNESS OF MIXING ZONE	[m]	Sampled
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled

$$DBOT = 10 \cdot - (DUNSAT + DMIX) \qquad \text{(below eqn. 3.8.5)}$$

Unit check: $[m] - ([m] + [m]) = [m]$

Note 1: Assumes tailings have a total depth of 10 [m].

Note 2: Equation (3.7.10) for DBOT is incorrect (SENES letter (1986-12-09)).

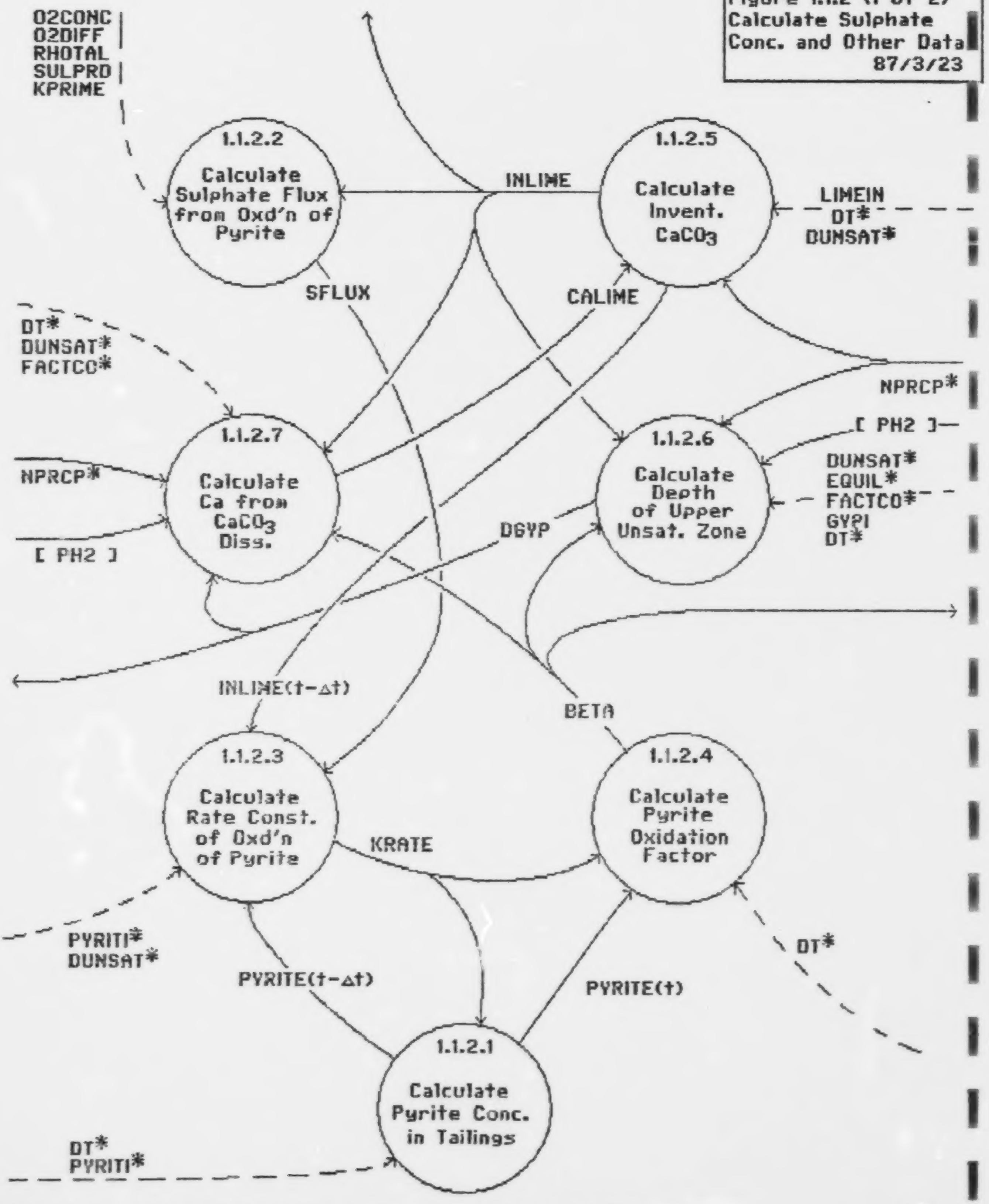
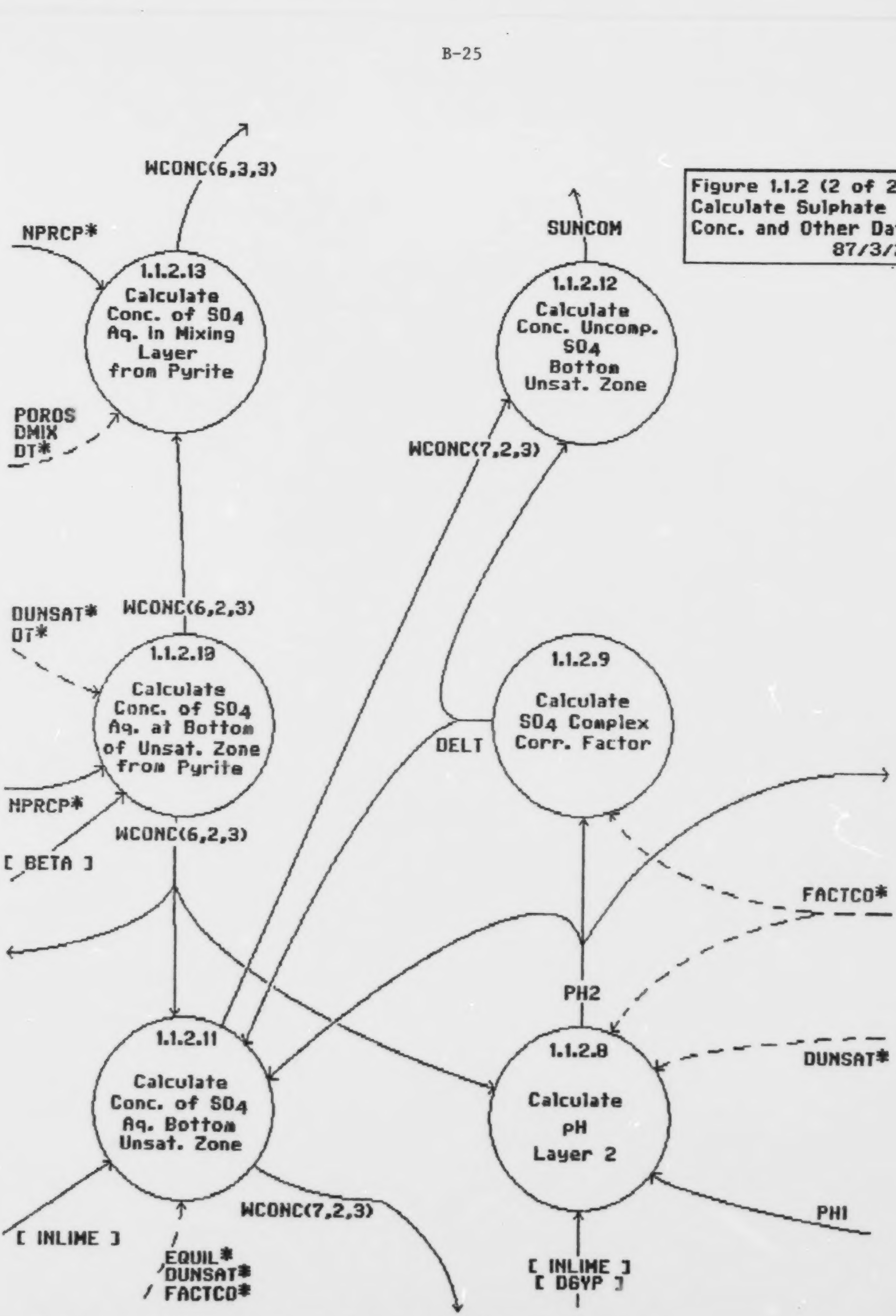

O2CONC
O2DIFF
RHOTAL
SULPRD
KPRIME
1.1.2.2
Calculate Sulphate Flux from Oxd'n of Pyrite
INLIME
1.1.2.5
Calculate Invent. CaCO3
LIMEIN
DT*
DUNSAT*
SFLUX
CALIME
DT*
DUNSAT*
FACTCO*
NPRCP*
1.1.2.7
Calculate Ca from CaCO3 Diss.
NPRCP*
[PH2]
[PH2]
1.1.2.6
Calculate Depth of Upper Unsat. Zone
DUNSAT*
EQUIL*
FACTCO*
GYPI
DT*
DGYP
INLIME(t-Δt)
BETA
1.1.2.3
Calculate Rate Const. of Oxd'n of Pyrite
1.1.2.4
Calculate Pyrite Oxidation Factor
KRATE
PYRITI*
DUNSAT*
DT*
PYRITE(t-Δt)
PYRITE(t)
1.1.2.1
Calculate Pyrite Conc. in Tailings
DT*
PYRITI*

Figure 1.1.2 (1 of 2)
Calculate Sulphate
Conc. and Other Data
87/3/23

Note: [X] indicates a variable X from part 2 of this figure.

Figure 1.1.2 (2 of 2)
Calculate Sulphate
Conc. and Other Data
87/3/23


WCONC(6,3,3)
NPRCP*
1.1.2.13
Calculate Conc. of SO4 Aq. in Mixing Layer from Pyrite
POROS
DMIX
DT*
SUNCOM
1.1.2.12
Calculate Conc. Uncomp. SO4 Bottom Unsat. Zone
WCONC(7,2,3)
DUNSAT*
DT*
WCONC(6,2,3)
1.1.2.10
Calculate Conc. of SO4 Aq. at Bottom of Unsat. Zone from Pyrite
NPRCP*
[BETA]
WCONC(6,2,3)
1.1.2.9
Calculate SO4 Complex Corr. Factor
DELT
FACTCO*
PH2
1.1.2.11
Calculate Conc. of SO4 Aq. Bottom Unsat. Zone
1.1.2.8
Calculate pH Layer 2
DUNSAT*
PH1
[INLIME]
WCONC(7,2,3)
EQUIL*
DUNSAT*
FACTCO*
[INLIME]
[DGYP]

Note: [X] indicates a variable from part 1 of this figure

Figure 1.1.2.1
Calculate PYRITE
CONC. IN TAILINGS
(PYRITE)

PYRITE - PYRITE CONC. IN TAILINGS [mol m^{-3}].
Concentration of pyrite in tailings
at TIME=t.

PYRITI
DT≡Δt - - -> PYRITE(t) <—— PYRITE(t-Δt)
KRATE

Short Name	Long Name	SI Unit	Source
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
KRATE	RATE CONST. OF OXD'N OF PYRITE	[a^{-1}]	1.1.2.3
PYRITE	PYRITE CONC. IN TAILINGS	[mol m^{-3}]	1.1.2.1
PYRITI	INIT. CONC. OF PYRITE IN TAILINGS	[mol m^{-3}]	Sampled

$$\text{PYRITE}(-\Delta t) = \text{PYRITI} \qquad \text{(eqn. 3.2.1)}$$

$$\text{PYRITE}(t) = \text{PYRITE}(t-\Delta t) * \text{EXP}(-\text{KRATE} * \text{DT})$$

$$\text{If PYRITE}(t) \leq 1.0 \times 10^{-6} \quad \text{PYRITE}(t) = 1.0 \times 10^{-6}$$

(eqn. 3.3.11 and below)

Unit check: $[\text{mol m}^{-3}] * [\text{EXP}([a^{-1}] * [a])] = [\text{mol m}^{-3}]$

Note 1: Inspection of the UTAP2 code shows that PYRITE(0) = PYRITI. (BWG 87-04-06)

Note 2: Inspection of the UTAP2 code shows that (for the lime option only) the second equation for PYRITE(t) is used only when KRATE $\leq$ 30/DT;otherwise PYRITE(t) = 1.0×10^{-6}. The other two equations always apply. This change has been implemented in SYVAC3-UT2. (BWG, 87-04-28)

SFLUX - SULPHATE FLUX FROM OXD'N OF PYRITE [mol m^{-2} a^{-1}]. Net sulphate flux out of the bottom of the unsaturated zone (and into the mixing zone) due to the oxidation of pyrite and the downward movement of water.

Figure 1.1.2.2
Calculate SULPHATE FLUX FROM OXD'N OF PYRITE (SFLUX)

O2CONC
O2DIFF
KPRIME - - -> SFLUX <—— INLIME
RHOTAL
SULPRD

Short Name	Long Name	SI Unit	Source
INLIME	INVENT. $CACO_3$	[mol m^{-3}]	1.1.2.5
KPRIME	RATIO OF KO_2 TO [O_2]	[-]	Sampled
O2CONC	O_2 CONC. IN AIR	[mol m^{-3}]	Sampled
O2DIFF	O_2 DIFFUSIVITY IN TAILINGS	[m^2 a^{-1}]	Sampled
RHOTAL	TAILINGS BULK DENSITY	[g m^{-3}]	Sampled
SFLUX	SULPHATE FLUX FROM OXD'N OF PYRITE	[mol m^{-2} a^{-1}]	1.1.2.2
SULPRD	SULPHATE PRODUCTION RATE	[mol g^{-1} a^{-1}]	Sampled

If INLIME ≤ 0

$$\text{SFLUX} = \left\{\frac{8}{7.5} * \text{SULPRD} * \text{RHOTAL} * \text{O2CONC} * \text{O2DIFF} * [1-K' * \ln \left(\frac{1+K'}{K'}\right)]\right\}^{1/2}$$

(eqn. 3.3.9
see Note 4)

If INLIME > 0

$$\text{SFLUX} = 0.05 * \left\{\frac{8}{7.5} * \text{SULPRD} * \text{RHOTAL} * \text{O2CONC} * \text{O2DIFF} * (1-K' * \ln \left(\frac{1+K'}{K'}\right)]\right\}^{1/2}$$

(eqn. 3.3.46)

Unit check: $\{[\text{mol g}^{-1}\ \text{a}^{-1}] * [\text{g m}^{-3}] * [\text{mol m}^{-3}] * [\text{m}^2\ \text{a}^{-1}] * [-]\}^{1/2}$
$= [\text{mol m}^{-2}\ \text{a}^{-1}]$

Note 1: The factors 8, 7.5 and 0.5 are assumed to be dimensionless.

Note 2: INLIME is not explicitly defined by SENES but is required to determine if $CaCO_3$ is still present at any particular time.

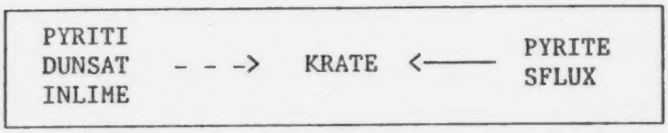
Note 3: In the above equations, K' is an abbreviation for KPRIME.

Note 4: Inspection of the UTAP2 code shows that condition (a) is applied as soon as INLIME is less than or equal to zero. (The condition is also ≤ 0, not $=0$). (BWG, 87-04-28)

Note 5: Inspection of the UTAP2 code shows that the approximate value 1.067 is used instead of 8/7.5. SYVAC3-UT2 was changed to use 1.067. (THA, 87-04-29)

KRATE - RATE CONST. OF OXD'N OF PYRITE [a^{-1}].
Rate constant for oxidation of pyrite.

Figure 1.1.2.3
Calculate RATE CONST.
OF OXD'N OF PYRITE
(KRATE)



Short Name	Long Name	SI Unit	Source
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
INLIME	INVENT. $CACO_3$	[mol m^{-3}]	1.1.2.5
KRATE	RATE CONST. OF OXD'N OF PYRITE	[a^{-1}]	1.1.2.3
PYRITE	PYRITE CONC. IN TAILINGS	[mol m^{-3}]	1.1.2.1
PYRITI	INIT. CONC. OF PYRITE IN TAILINGS	[mol m^{-3}]	Sampled
SFLUX	SULPHATE FLUX FROM OXD'N OF PYRITE	[mol m^{-2} a^{-1}]	1.1.2.2

$$\text{KRATE} = \frac{\text{SFLUX}}{2 * \text{DUNSAT} * \text{PYRITI}}$$

(eqn. 3.3.10; see Note 2)

Unit check: [mol m^{-2} a^{-1}] / [m] * [mol m^{-3}] = [a^{-1}]

Note 1: The parameter "2" is dimensionless.

Note 2: Inspection of the UTAP2 code shows that the following logic is used:

```
if (t ≤ 0)                          [initial condition]
     KRATE is calculated from eqn. (3.3.10)
else if (INLIME(0) ≤ 0 or INLIME(t-Δt) > 0)
                                    [no lime added, or lime remains]
     KRATE(t) = KRATE(t-Δt)
else if (INLIME(t-2Δt) > 0 and INLIME(t-Δt) ≤ 0)
                                    [depletion of added lime]
     KRATE(t) is calculated from a modified form of eqn. (3.3.10)
     in which PYRITI has been replaced by PYRITE(t-Δt)
else KRATE(t) = KRATE(t-Δt)
```

SYVAC3-UT2 has been adapted to use this logic. (THA, 87-04-30)

Figure 1.1.2.4
Calculate PYRITE
OXIDATION FACTOR
(BETA)

BETA - PYRITE OXIDATION FACTOR [mol m^{-3}]. Number of moles of pyrite oxidized per unit volume between TIME=t-Δt and TIME=t.

DT≡Δt - - -> BETA <—— PYRITE (t-Δt)
KRATE

Short Name	Long Name	SI Unit	Source
BETA	PYRITE OXIDATION FACTOR	[mol m^{-3}]	1.1.2.4
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
KRATE	RATE CONST. OF OXD'N OF PYRITE	[a^{-1}]	1.1.2.3
PYRITE	PYRITE CONC. IN TAILINGS	[mol m^{-3}]	1.1.2.1

$$\text{BETA} = \text{PYRITE}(t-\Delta t) * [1 - \text{EXP}(-\text{KRATE} * \text{DT})] \qquad \text{(below eqn. 3.3.22)}$$

Unit check: EXP: ([a^{-1}] * [a]) = [-]
BETA: [mol m^{-3}] * [-] = [mol m^{-3}]

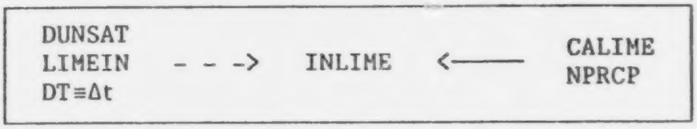
Note 1: Units for BETA incorrectly given as [-] in Table A.3.

Note 2: PYRITE(-Δt) ≡ PYRITI, and BETA is not required or defined for t=-Δt.

Note 3: Inspection of the UTAP2 code shows that (for the lime option only), the above equation for BETA is used only when KRATE $\leq$ 30/DT; otherwise BETA = PYRITE(t-Δt). This change has been implemented in SYVAC3-UT2. (BWG, 87-04-28)

Figure 1.1.2.5
Calculate
INVENT. $CACO_3$
(INLIME)

INLIME - INVENT. $CACO_3$ [mol m^{-3}]. The residual concentration of limestone or calcite (as $CaCO_3$) in the unsaturated layer at time t.



Short Name	Long Name	SI Unit	Source
CALIME	CA FROM $CACO_3$ DISS.	[mol m^{-3}]	1.1.2.7
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
INLIME	INVENT. $CACO_3$	[mol m^{-3}]	1.1.2.5
LIMEIN	INIT. CONC. LIMESTONE	[mol m^{-3}]	1.1.1.3
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled

$$\text{INLIME} \equiv 0.0 \quad \text{if} \quad \text{LIMEIN} = 0$$

$$\text{INLIME} = \text{LIMEIN at TIME} = -\Delta t \quad \text{(Note 1)}$$

Else

$$\text{INLIME} = \quad \text{LIMEIN} - \frac{\Sigma(\text{CALIME} * \text{NPRCP} * \text{DT})}{\text{DUNSAT}} \qquad \text{(see Notes 2 and 4)}$$

where the summation is over all time intervals (Δt) to TIME=t

Unit check:

$$[\text{mol m}^{-3}] - \frac{[\text{mol m}^{-3}] * [\text{m a}^{-1}]\ [\text{a}]}{[\text{m}]} = [\text{mol m}^{-3}]$$

Note 1: By definition of the scenario; see SENES section 2.7.

Note 2: The parameter INLIME is not specifically defined in SENES Vol. 3 but is defined from equation (3.3.70). The summation is over all time steps to time t.

Note 3: SENES has used C for C_{λ_w} (eqn 3.3.67) and $[Ca\ CO_3]° = CaCO_3^\circ$ (eqn. 3.3.70 and Appendix A.3).

Note 4: Inspection of the UTAP2 code shows that the factor DUNSAT does not appear in the calculation of INLIME. It has been removed from SYVAC3-UT2, even though it is needed to pass the unit check. (BWG, 87-04-28)

Figure 1.1.2.6
Calculate DEPTH OF
UPPER UNSAT. ZONE
(DGYP) (Pg. 1 of 2)

DGYP - DEPTH OF UPPER UNSAT. ZONE [m]. Depth of the gypsum depleted (upper) portion of the unsaturated zone.

DUNSAT - - -> DGYP(t) <—— DGYP(t=Δt)
DELTAH

DT≡Δt
EQUIL
DUNSAT - - -> DELTAH <—— DGYP(t-Δt)
GYPI
FACTCO

DGYP(t-Δt)
INLIME
NPRCP
PH2
BETA

Short Name	Long Name	SI Unit	Source
BETA	PYRITE OXIDATION FACTOR	$[\mathrm{mol\ m^{-3}}]$	1.1.2.4
DELTAH	INCREMENTAL CHANGE IN DGYP	[m]	(1.1.2.6)
DGYP	DEPTH OF UPPER UNSAT. ZONE	[m]	1.1.2.6
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
EQUIL	SQ. ROOT OF EQBM. CONST. GYPSUM	$[\mathrm{mol\ m^{-3}}]$	1.1.1.2
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
GYPI	INIT. GYPSUM CONTENT IN TAILINGS	$[\mathrm{mol\ m^{-3}}]$	1.1.1.1
INLIME	INVENT. $CACO_3$	$[\mathrm{mol\ m^{-3}}]$	1.1.2.5
NPRCP	NET PRECIPITATION	$[\mathrm{m\ a^{-1}}]$	Sampled
PH2	PH LAYER 2	[-]	1.1.2.8

For t>0

(a) If DGYP (t-Δt) = DUNSAT
Then DELTAH = 0.0 (and DGYP(t) = DUNSAT)

(b) If DGYP(t-Δt) < DUNSAT and INLIME(t-Δt) = 0.0 then

$$\mathrm{DELTAH} = \left[\frac{(\mathrm{BETA} * \mathrm{DGYP}(t-\Delta t))^2}{(\mathrm{GYPI} + \mathrm{BETA})^2} + \frac{(\mathrm{NPRCP} * \mathrm{DT} * \mathrm{EQUIL})^2}{\mathrm{GYPI} * (\mathrm{GYPI} + \mathrm{BETA})}\right]^{0.5} - \frac{\mathrm{BETA} * \mathrm{DGYP}(t-\Delta t)}{(\mathrm{GYPI} + \mathrm{BETA})}$$

(eqn. 3.3.26; see Note 6)

(c) If DGYP(t-Δt) < DUNSAT and INLIME(t-Δt) > 0.0 then

$$\mathrm{DELTAH} = \frac{1}{\mathrm{GYPI}}\left\{1000*\left(\frac{10^{(2*\mathrm{PH2}-16.47)}}{\mathrm{FACTCO}} - 10^{-4}\right) * \mathrm{NPRCP} * \mathrm{DT} - 2 * \mathrm{DGYP}(t-\Delta t) * \mathrm{BETA}\right\}$$

(eqn. 3.3.65)
(see Note 3)

$$\mathrm{DGYP}(t) = \mathrm{DGYP}(t-\Delta t) + \mathrm{DELTAH}$$

(eqn. 3.3.28)

If [DGYP(t-Δt) + DELTAH] > DUNSAT then
DGYP(t) = DUNSAT

For t=0, DGYP(t)=0 (see Note 5)

Unit check:

DELTAH (b)
$$\left[\frac{[\mathrm{mol\ m^{-3}}]^2 * [\mathrm{m}]^2}{([\mathrm{mol\ m^{-3}}] + [\mathrm{mol\ m^{-3}}])^2} + \frac{[\mathrm{m\ a^{-1}}]^2 * [\mathrm{a}]^2 * [\mathrm{mol\ m^{-3}}]^2}{[\mathrm{mol\ m^{-3}}] * ([\mathrm{mol\ m^{-3}}] + [\mathrm{mol\ m^{-3}}])}\right]^{0.5} - \frac{[\mathrm{mol\ m^{-3}}] * [\mathrm{m}]}{([\mathrm{mol\ m^{-3}}] + [\mathrm{mol\ m^{-3}}])} = [\mathrm{m}]$$

Figure 1.1.2.6
Calculate DEPTH OF
UPPER UNSAT. ZONE
(DGYP) (Pg. 2 of 2)

(c) $$\frac{1}{[\text{mol m}^{-3}]} * \left\{[\text{dm}^3\ \text{m}^{-3}] * \left(\frac{[\text{mol dm}^{-3}]}{[-]} - [\text{mol dm}^{-3}]\right) * [\text{m a}^{-1}] * [\text{a}] - [\text{m}] * [\text{mol m}^{-3}]\right\} = [\text{m}]$$

DGYP $[\text{m}] + [\text{m}] = [\text{m}]$

Note 1: The expression for BETA (near eqn 3.3.22) has been used to modify (simplify) these expressions.

Note 2: DGYP(-Δt) = 0 by definition (also see SENES pg 3-3).

Note 3: The pH used in equation 3.3.6.5 is pH2, as confirmed in a letter from SENES (1986-11-04, item 39).

Note 4: The factor of 1000 $[\text{dm}^3\ \text{m}^{-3}]$ is required in (c) to convert the concentration to $[\text{mol m}^{-3}]$.

Note 5: The initial condition was taken from the UTAP2 code. (BWG, 87-03-30)

Note 6: Inspection of the UTAP2 code shows that the following logic is used for t > 0.

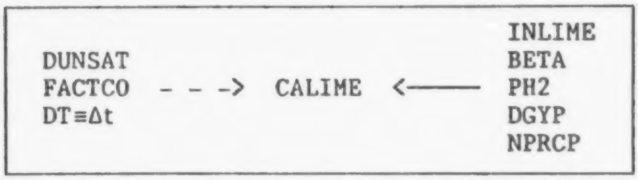
```
If (DGYP(t-Δt) $\geq$ DUNSAT)          [gypsum depleted]
   DELTAH = 0
   DGYP(t) = DGYP(t-Δt)
else if (INLIME(0) $\leq$ 0)           [no lime added]
   DELTAH is calculated using eqn. (3.3.26)
   DGYP(t) = DGYP(t-Δt) + DELTAH
else if (INLIME(t-Δt) $\leq$ 0)        [lime added, but depleted]
   DELTAH is calculated from a modified form of eqn. (3.3.26), in
   which the term BETA * DGYP(t-Δt) is doubled in the two places
   it appears.
   e.g. the first term becomes: $\frac{(2 * BETA * DGYP(t-\Delta t))^2}{(GYPI + BETA)^2}$

   DGYP(t) = DGYP(t-Δt) + DELTAH
else                                   [lime added, some remains]
   DELTAH is calculated using eqn. (3.3.65)
   DGYP(t) = DGYP(t-Δt) + DELTAH
if (DGYP(t) > DUNSAT) DGYP(t) = DUNSAT
```

SYVAC3-UT2 has been adapted to use this logic.
(THA, 87-04-30)

Figure 1.1.2.7
Calculate CA FROM $CACO_3$ DISS.
(CALIME)

CALIME - CA FROM $CACO_3$ DISS. [mol m^{-3}]. Average solution concentration of calcium at the bottom of the unsaturated layer, between TIME=t-Δt and TIME=t and attributable to the dissolution of $CaCO_3$.



Short Name	Long Name	SI Unit	Source
BETA	PYRITE OXIDATION FACTOR	[mol m^{-3}]	1.1.2.4
CALIME	CA FROM $CACO_3$ DISS.	[mol m^{-3}]	1.1.2.7
DGYP	DEPTH OF UPPER UNSAT. ZONE	[m]	1.1.2.6
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
INLIME	INVENT. $CACO_3$	[mol m^{-3}]	1.1.2.5
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled
PH2	PH LAYER 2	[-]	1.1.2.8

$$\text{CALIME} = 0.0 \qquad \text{if} \quad \text{INLIME}(t-\Delta t) = 0.0 \qquad \text{(see Note 4)}$$

$$\text{CALIME} = 0.0 \qquad \text{at } t=-\Delta t \text{ if LIMEIN} = 0.0$$

If DGYP < DUNSAT

$$\text{CALIME} = 1000 * \left(\frac{10^{(11.87-2*PH2)} - 10^{(2*PH2-16.47)}}{\text{FACTCO}} + 0.8 \times 10^{-4} \right) + \frac{2 * \text{DUNSAT} * \text{BETA}}{\text{NPRCP} * \text{DT}}$$

(eqn. 3.3.68; see Note 3)

If DGYP ≥ DUNSAT

$$\text{CALIME} = 1000 * \left(\frac{10^{(11.87-2*PH2)}}{\text{FACTCO}} - 0.2 * 10^{-4} \right)$$

(eqn. 3.3.69; see Note 2)

Unit check:

$$\frac{[\text{m}] * [\text{mol m}^{-3}]}{[\text{m a}^{-1}] * [\text{a}]} = [\text{mol m}^{-3}]$$

(last term for eqn.(3.3.68) only)

Note 1: The expression for BETA (near equation 3.3.22) has been used to modify (simplify) the expression.

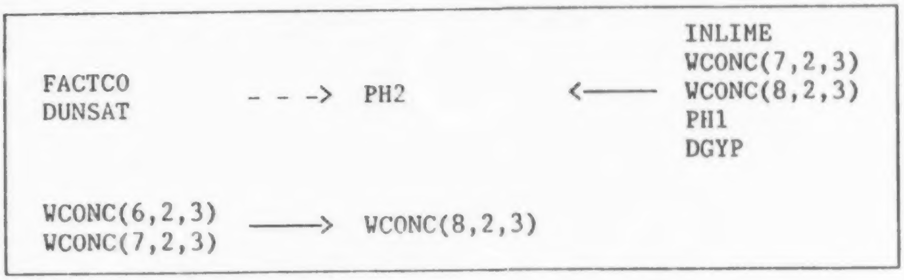
Note 2: Equations 3.3.68 and 3.3.69 have been modified according to SENES letter (1986-12-09).

Note 3: Inspection of the UTAP2 code shows that the factor 11.86 is used instead of 11.87 in two places. (BWG, 87-04-28)

Note 4: Inspection of the UTAP2 code gives no indication that CALIME=0 when lime is not present. However this condition appears to be correct (and possibly not required) and so has been left in SYVAC3-UT2. (BWG, 87-04-28)

PH2 - PH LAYER 2 [-]. The pH of the solution in the gypsum-containing layer of the unsaturated zone of the tailings.

Figure 1.1.2.8
Calculate
PH LAYER 2
(PH2)
(Page 1 of 4)



Short Name	Long Name	SI Unit	Source
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
DGYP	DEPTH OF UPPER UNSAT. ZONE	[m]	1.1.2.6
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
INLIME	INVENT. $CACO_3$	[mol m^{-3}]	1.1.2.5
PH1	PH LAYER 1	[-]	1.1.3.2
PH2	PH LAYER 2	[-]	1.1.2.8
WCONC(6,2,3)	CONC. OF SO_4 AQ. AT BOTTOM OF UNSAT. ZONE FROM PYRITE	[mol m^{-3}]	1.1.2.10
WCONC(7,2,3)	CONC. OF SO_4 AQ. BOTTOM UNSAT. ZONE	[mol m^{-3}]	1.1.2.11
WCONC(8,2,3)	CONC. OF CA AQ. BOTTOM UNSAT. ZONE	[mol m^{-3}]	(1.1.2.8)

(a) If INLIME ≠ 0.0, PH2 is calculated iteratively from:

$$2*\left(\frac{10^{(11.87-2*PH2)}}{FACTCO}\right) + 10^{(0.3-PH2)} = 2*\left(\frac{10^{(2*PH2-16.47)}}{FACTCO}\right) + \left(\frac{10^{(PH2-9.73)}}{FACTCO^{0.25}}\right)$$

(eqn. 3.6.25; see Note 7 & 8)

(b) If INLIME = 0.0, PH2 is calculated iteratively from the equation for WCONC(8,2,3):

$$WCONC(8,2,3) = WCONC(7,2,3) - WCONC(6,2,3)$$

(eqns. 3.3.39 & 3.3.40; see Note 8)

and

$$3*\left(\frac{10^{6.5}}{(FACTCO)^{2.25}} + 10^{5.97}\right) * 10^{-3*PH2} + 2*\left(\frac{10^{1.53}}{FACTCO} + 10^{3.78}\right) * 10^{-2*PH2}$$
$$+ \left(10^{0.3} + \frac{1}{(FACTCO)^{0.25}}\right) * 10^{-PH2} + 2 * WCONC(8,2,3) * 10^{-3}$$
$$= \frac{10^{PH2-11.27}}{(FACTCO)^{0.25}} + 10^{-3} * WCONC(7,2,3)$$
$$* \left(\frac{2 - (FACTCO)^{0.75} * 10^{(9.7-3*PH2)} - (FACTCO)^{3} * 10^{(8.99-3*PH2)}}{1 + (FACTCO)^{0.75} * 10^{(9.7-3*PH2)} + (FACTCO)^{3} * 10^{(8.99-3*PH2)}}\right)$$

(eqn. 3.6.23; see Notes 3 to 5)

Unit check: WCONC(8,2,3): [mol m^{-3}] - [mol m^{-3}] = [mol m^{-3}]

(a) [-] all terms have units [mol dm^{-3}], pH2 is dimensionless.
(b) Unit check failure. WCONC(7,2,3) and WCONC(8,2,3) are in [mol m^{-3}]. Other terms are [mol dm^{-3}]. The terms containing WCONC(7,2,3) and WCONC(8,2,3) have been multiplied by 10^{-3} [m^3 dm^{-3}] to eliminate the inconsistency. PH2 is, of course, dimensionless.

Figure 1.1.2.8
Calculate
PH LAYER 2
(PH2)
(Page 2 of 4)

Note 1: The expression for WCONC(8,2,3) is derived from the fact that equation (3.3.40) only differs from (3.3.39) by an additive term: $[SO_4^{2-}]_{p,\lambda_w}$.

Note 2: It is assumed $[SO_4^{2-}]_{T,\lambda_w} = [SO_4^{2-}]_{\lambda_w}$.

Note 3: Inspection of the UTAP2 code shows that WCONC(6,2,3) is used instead of WCONC(7,2,3), and the factor $10^{8.97}$ instead of $10^{8.99}$ (in two places). Both modifications are used in SYVAC3-UT2 (BWG, 87-04-02).

Note 4: Inspection of the UTAP2 code shows that the term: 2 * WCONC(8,2,3) * 10^{-3} is replaced with 2 * CA2 where

$$CA2 = [10^{-4.6} * (1 + FACTCO^{0.75} * 10^{9.7-3*PH2} + FACTCO^{3} * 10^{8.97-3*PH2}) / FACTCO^{2} + \tfrac{1}{4}CS^{2}]^{0.5} - 0.5 * CS$$

and CS = WCONC(6,2,3) / 1000

Furthermore the term 10^{-3} * WCONC(7,2,3) * {...} is replaced with (CA2 + CS) * {...}. Both of these changes have been implemented in SYVAC3-UT2. (THA, 87-04-20)

Note 5: Inspection of the UTAP2 code shows that, once gypsum has been depleted from Layer 2 (i.e. DGYP $\geq$ DUNSAT), PH2 = PH1. (BWG, 87-04-27)

Note 6: The original specifications had WCONC(7,2,3), DELT and PH2 in an iterative loop. However with the use of WCONC(6,2,3) instead of WCONC(7,2,3), the iteration structure is no longer required. In particular, DFD 1.1.2 no longer requires a link between bubble 1.1.2.11 and 1.1.2.8. These comments are a reflection of the UTAP2 code and in contradiction to response 68 from SENES (in a letter dated 1986 Dec. 9). (BWG, 87-04-28)

Note 7: Inspection of the UTAP2 code shows some variance in the calculation of PH2 to the equations given above for the lime option. They are:

(1) When gypsum has been depleted from the unsaturated zone (i.e. DGYP $\geq$ DUNSAT) PH2 = PH1 where PH1 is calculated using
    (a) the INLIME=0 option when the lime has also been depleted
    (b) the INLIME>0 option when the lime has not been depleted.
    (See DDD 1.1.3.2 for calculation of PH1.)
(2) When gypsum is present and lime depleted, then equation (3.6.23) is appropriate.
(3) When gypsum and lime are present,
    PH2 = PH2LIM
    where PH2LIM is the (time-independent) solution to equation (3.6.25) given above.

All calculations for PH2 (with the lime options) are done before all other calculations of sulphate and calcium concentrations, and PH2 is not recalculated (during any given time step). These changes are implemented in SYVAC3-UT2. (BWG, 87-04-28)

Note 8: Inspection of the UTAP2 code shows that, for the lime option, when gypsum and lime are present (or when gypsum is absent but lime is present):

$$WCONC(8,2,3) = 1000 * 10^{(11.86-2*PH2)} / FACTCO.$$

When there is no gypsum and no lime present, WCONC(8,2,3) = 0.0. It is not clear if this variable is used elsewhere; however it has been included in options (a) and (b) above. (BWG, 87-04-28)

Note 9: Inspection of the UTAP2 code shows that the following logic is used:

(a) $(t \leq 0)$ [initial condition]
if (INLIME(0) > 0)
PH2 is calculated iteratively as the solution to eqn. (3.6.25). else
PH2 is calculated iteratively as the solution to eqn. (3.6.23a) below

(b) $(t>0)$ and INLIME(0) ≤ 0 [no lime added]
if (DGYP(t) $\geq$ DUNSAT) [gypsum depleted]
PH2 is calculated iteratively as the solution to the following equation (normally used to calculate PH1; see other notes in DDD 1.1.3.2):

$$\frac{10^{-PH2}}{(FACTCO)^{0.25}} + 3\left(\frac{10^{6.5}}{(FACTCO)^{2.25}} + 10^{5.97}\right)10^{-3*PH2} + 2\left(\frac{10^{1.53}}{FACTCO} + 10^{3.78}\right)$$

$$* \; 10^{-2*PH2} + 10^{(0.3-PH2)} = \frac{WCONC(7,1,3)}{1000}$$

$$* \left(\frac{2-(FACTCO)^{0.75}*(10^{(9.7-3*PH2)})-(FACTCO)^{3}*(10^{(8.99-3*PH2)})}{1+(FACTCO)^{0.75}*(10^{(9.7-3*PH2)})+(FACTCO)^{3}*(10^{(8.99-3*PH2)})}\right) + \left(\frac{10^{(PH2-11.27}}{FACTCO^{0.25}}\right)$$

else [gypsum still present]
PH2 is calculated iteratively as the solution to the following modified form of eqn. (3.6.23):

$$3 * \left(\frac{10^{6.5}}{FACTCO^{2.25}} + 10^{5.97}\right) * 10^{(-3*PH2)} + 2 * \left(\frac{10^{1.53}}{FACTCO} + 10^{3.78}\right) * 10^{(-2*PH2)}$$

$$+ \left(10^{0.3} + \frac{1}{FACTCO^{0.25}}\right) * 10^{-PH2} + 2 * CA2 = \frac{10^{(PH2-11.27)}}{FACTCO^{0.25}} + (CA2 + CS)$$

$$* \left(\frac{2 - FACTCO^{0.75} * 10^{(9.7-3*PH2)} - FACTCO^{3} * 10^{(8.97-3*PH2)}}{1 + FACTCO^{0.75} * 10^{(9.7-3*PH2)} + FACTCO^{3} * 10^{(8.97-3*PH2)}}\right)$$

(eqn. 3.6.23a)

where

$$CA2 = \left[10^{-4.6} * (1 + FACTCO^{0.75} * 10^{(9.7-3*PH2)} + FACTCO^{3}\right.$$

$$\left. * \; 10^{(8.97-3*PH2)}) \; / \; FACTCO^{2} + \frac{CS^{2}}{4}\right]^{0.5} - \frac{CS}{2}$$

and $CS = WCONC(6,2,3) \; / \; 1000$

Figure 1.1.2.8
Calculate
PH LAYER 2
(PH2)
(Page 4 of 4)

```
(c) (t>0) and INLIME(0)>0              [lime was added]
    if (DGYP(t-Δt) ≥ DUNSAT            [gypsum was depleted last time
                                        step] and
    if (INLIME(t-Δt) > 0)              [lime still present last time
                                        step]
    PH2 is calculated iteratively as the solution to the following
    equation (normally used to calculate PH1; see other notes in DDD
    1.1.3.2).
```

$$2\left(\frac{10^{(11.87-2*PH2)}}{FACTCO}\right) + 10^{(0.3-PH2)} = \frac{2*WCONC(7,1,3)}{1000} + \frac{10^{(PH2-9.73)}}{(FACTCO)^{0.25}}$$

```
    else                               [lime depleted by last time
                                        step]
    PH2 is calculated iteratively as the solution to eqn. (3.6.17).
    else if (INLIME(t-Δt) > 0)         [both gypsum and lime remained
                                        last time step]
    PH2 is calculated iteratively from eqn. (3.6.25)
    else                               [gypsum remained last
                                        time step, lime didn't]
        PH2 is calculated iteratively from eqn. (3.6.23a) above.
```

SYVAC3-UT2 has also been adapted to use this logic.
(THA, 87-05-04)

Figure 1.1.2.9
Calculate SO_4 COMPLEX
CORR. FACTOR
(DELT)

DELT - SO_4 COMPLEX CORR. FACTOR [-]. Factor (dependent on pH) to obtain the free sulphate concentration from the total sulphate concentration.

FACTCO - - -> DELT <—— PH2

Short Name	Long Name	SI Unit	Source
DELT	SO_4 COMPLEX CORR. FACTOR	[-]	1.1.2.9
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
PH2	PH LAYER 2	[-]	1.1.2.8

$$DELT = 1 + (FACTCO)^{3} * 10^{(8.99-3*PH2)} + (FACTCO)^{0.75} * 10^{(9.7-3*PH2)}$$

(eqn. 3.3.38)

Unit check: dimensionless

Note 1: DELT is involved in an iterative calculation with WCONC(7,2,3) and PH2 if DGYP<DUNSAT and INLIME=0.

Note 2: Subsequent inspection of the UTAP2 code reveals, however, that the iterative calculation is not required as PH2 does not use WCONC(7,2,3). More details are given in DDD 1.1.2.8. (BWG, 87-04-28)

Figure 1.1.2.10
Calculate CONC. OF SO_4 AQ. AT BOTTOM OF UNSAT. ZONE FROM PYRITE (WCONC(6,2,3))

WCONC(6,2,3) - CONC. OF SO_4 AQ. AT BOTTOM OF UNSAT. ZONE FROM PYRITE [mol m^{-3}]. Concentration of sulphate ions in the aqueous phase at the bottom of the unsaturated zone due to pyrite oxidation and downward movement of water (including sulphate in precipitation), as a function of time.

$$\begin{tikzcd}
\mathrm{DT} \equiv \Delta t \\ \mathrm{DUNSAT} \arrow[r, dashed] & \mathrm{WCONC}(6,2,3) & \mathrm{NPRCP} \arrow[l] \\ & & \mathrm{BETA}
\end{tikzcd}$$

Short Name	Long Name	SI Unit	Source
BETA	PYRITE OXIDATION FACTOR	[mol m^{-3}]	1.1.2.4
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled
WCONC(6,2,3)	CONC. OF SO_4 AQ. AT BOTTOM UNSAT. ZONE FROM PYRITE	[mol m^{-3}]	1.1.2.10

$$\mathrm{WCONC}(6,2,3) = \frac{2.0 * \mathrm{DUNSAT} * \mathrm{BETA}}{\mathrm{NPRCP} * \mathrm{DT}} + 0.1$$

(eqn. 3.3.14; see Notes 3 and 4)

Unit check:

$$\frac{[\mathrm{m}] * [\mathrm{mol\ m}^{-3}]}{[\mathrm{m\ a}^{-1}] * [\mathrm{a}]} + [\mathrm{mol\ m}^{-3}] = [\mathrm{mol\ m}^{-3}]$$

Note 1: This formulation includes the term "0.1" from precipitation and may not be appropriate to all calculations. In the WATEX module 0.071 is used instead of 0.1 [mol m^{-3}].

Note 2: BETA, defined near (3.3.22), is used to simplify the expression.

Note 3: The initial condition, from eqn. (3.2.3), is the same as eqn. (3.3.14) except that the term 0.1 is omitted (BWG, 87-04-02).

Note 4: Inspection of the UTAP2 code shows that WCONC(6,2,3) is reset to 1.0D-20 if its computed value is equal to zero. This option was implemented in SYVAC3-UT2. (BWG, 87-04-28)

Figure 1.1.2.11
Calculate CONC. OF SO_4
AQ. BOTTOM UNSAT. ZONE
(WCONC(7,2,3))
(Page 1 of 2)

WCONC(7,2,3) - CONC. OF SO_4 AQ. BOTTOM UNSAT. ZONE $[\text{mol m}^{-3}]$. The total concentration of sulphate ions in the aqueous phase at the bottom of the saturated layer.

DUNSAT
EQUIL - - -> WCONC(7,2,3) <—— DGYP
FACTCO
PH2
DELT
WCONC(6,2,3)
INLIME

Short Name	Long Name	SI Unit	Source
DELT	SO_4 COMPLEX CORR. FACTOR	[-]	1.1.2.9
DGYP	DEPTH OF UPPER UNSAT. ZONE	[m]	1.1.2.6
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
EQUIL	SQ. ROOT OF EQBM. CONST. GYPSUM	$[\text{mol m}^{-3}]$	1.1.1.2
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
INLIME	INVENT. $CACO_3$	$[\text{mol m}^{-3}]$	1.1.2.5
PH2	PH LAYER 2	[-]	1.1.2.8
WCONC(6,2,3)	CONC. OF SO_4 AQ. AT BOTTOM OF UNSAT. ZONE FROM PYRITE	$[\text{mol m}^{-3}]$	1.1.2.10
WCONC(7,2,3)	CONC. OF SO_4 AQ. BOTTOM UNSAT. ZONE	$[\text{mol m}^{-3}]$	1.1.2.11

If

(a) DGYP = DUNSAT

$$\text{WCONC}(7,2,3) = \text{WCONC}(6,2,3) \qquad \text{(eqn. 3.3.43)}$$

(b) DGYP < DUNSAT and INLIME = 0

$$\text{WCONC}(7,2,3) = \left\{(\text{EQUIL})^2 * \text{DELT} + 0.25 * (\text{WCONC}(6,2,3))^2\right\}^{0.5} + 0.5 * (\text{WCONC}(6,2,3)) \qquad \text{(eqn. 3.3.40)}$$

(c) DGYP < DUNSAT and INLIME > 0

$$\text{WCONC}(7,2,3) = 1000 * \frac{10^{(2*\text{PH2}-16.47)}}{\text{FACTCO}} \qquad \text{(eqn. 3.3.60)}$$

Unit check:
(a) $[\text{mol m}^{-3}] = [\text{mol m}^{-3}]$
(b) $([\text{mol m}^{-3}]^2 + [\text{mol m}^{-3}]^2)^{0.5} + [\text{mol m}^{-3}] = [\text{mol m}^{-3}]$
(c) $[\text{dm}^3\ \text{m}^{-3}] * [\text{mol dm}^{-3}] = [\text{mol m}^{-3}]$

Note 1: Case (b) requires an iterative calculation of PH2, DELT and WCONC(7,2,3).

Note 2: EQUIL, defined near equation (3.3.22), has been used to modify (simplify) equation (3.3.40).

Figure 1.1.2.11
Calculate CONC. OF SO_4
AQ. BOTTOM UNSAT. ZONE
(WCONC(7,2,3))
(Page 2 of 2)

Note 3: Subsequent inspection of the UTAP2 code shows that WCONC(7,2,3), DELT and PH2 are not calculated iteratively. See DDD 1.1.2.8 for more details. (BWG, 87-04-28)

Note 4: Inspection of the UTAP2 code shows that the following logic is used:

```
if (t≤0)                                [initial condition]
    if (INLIME(0) > 0)
    WCONC(7,2,3) is calculated according to eqn. (3.3.60)
    else WCONC(7,2,3) is calculated from eqn. (3.3.40)
else if (INLIME(0) ≤ 0)                 [no lime added]
    if (DGYP(t) ≥ DUNSAT)               [gypsum depleted]
    WCONC(7,2,3) = WCONC(6,2,3)
else                                    [gypsum remains]
    WCONC(7,2,3) is calculated from eqn. (3.3.40)
else if (DGYP(t) ≥ DUNSAT)              [lime added, gypsum depleted]
    WCONC(7,2,3) = WCONC(6,2,3)
else if (INLIME(t-Δt) > 0)              [gypsum remains, lime remained
                                         last time step]
    WCONC(7,2,3) is calculated from eqn. (3.3.60)
else                                    [gypsum remains, lime depleted
                                         by last time step]
    WCONC(7,2,3) is calculated from eqn. (3.3.40)
```

SYVAC3-UT2 has been adapted to use this logic, which is similar (but not identical) to that described in the original specifications. (THA, 87-05-04)

Figure 1.1.2.12
Calculate CONC. UNCOMP. SO_4 BOTTOM UNSAT. ZONE (SUNCOM)

SUNCOM - CONC. UNCOMP. SO_4 BOTTOM UNSAT. ZONE [mol dm^{-3}]. Total concentration of uncomplexed sulphate ion at the bottom of the unsaturated zone.

WCONC(7,2,3)
DELT ——> SUNCOM

Short Name	Long Name	SI Unit	Source
DELT	SO_4 COMPLEX CORR. FACTOR	[-]	1.1.2.9
SUNCOM	CONC. UNCOMP. SO_4 BOTTOM UNSAT. ZONE	[mol dm^{-3}]	1.1.2.12
WCONC(7,2,3)	CONC. OF SO_4 AQ. BOTTOM UNSAT. ZONE	[mol m^{-3}]	1.1.2.11

SUNCOM = WCONC(7,2,3) / (DELT * 1000.) (eqn. 3.3.41)

Unit check: [mol m^{-3}] / ([-] * [dm^3 m^{-3}]) = [mol dm^{-3}]

Note: The factor of 1000 [dm^3 m^{-3}] is required to convert WCONC(7,2,3) to [mol dm^{-3}].

Figure 1.1.2.13
Calculate CONC. OF SO_4 AQ. IN MIXING LAYER FROM PYRITE (WCONC(6,3,3))

WCONC(6,3,3) - CONC. OF SO_4 AQ. IN MIXING LAYER FROM PYRITE [mol m^{-3}]. Concentration of sulphate ions in the aqueous phase in the mixing layer of the saturated zone due to pyrite oxidation and downward movement of water (including sulphate in precipitation), as a function of time.

DMIX
DT≡Δt - - -> WCONC(6,3,3) <—— WCONC(6,2,3)
POROS
WCONC(6,3,2)
NPRCP

Short Name	Long Name	SI Unit	Source
DMIX	THICKNESS OF MIXING ZONE	[m]	Sampled
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled
POROS	TAILINGS POROSITY	[-]	Sampled
WCONC(6,2,3)	CONC. OF SO_4 AQ. AT BOTTOM OF UNSAT. ZONE FROM PYRITE	[mol m^{-3}]	1.1.2.10
WCONC(6,3,2)	CONC. OF SO_4 AQ. IN MIXING LAYER FROM PYRITE (at TIME=(t-Δt))	[mol m^{-3}]	(1.1.2.13)
WCONC(6,3,3)	CONC. OF SO_4 AQ. IN MIXING LAYER FROM PYRITE (at TIME=t)	[mol m^{-3}]	1.1.2.13

Calculated from the finite difference equation

$$\text{WCONC}(6,3,3) = \text{WCONC}(6,2,3) + (\text{WCONC}(6,3,2) - \text{WCONC}(6,2,3)) * \text{EXP}\left[-\frac{\text{NPRCP} * \text{DT}}{\text{POROS} * \text{DMIX}}\right] \qquad \text{(eqn. 3.4.5)}$$

Unit check:

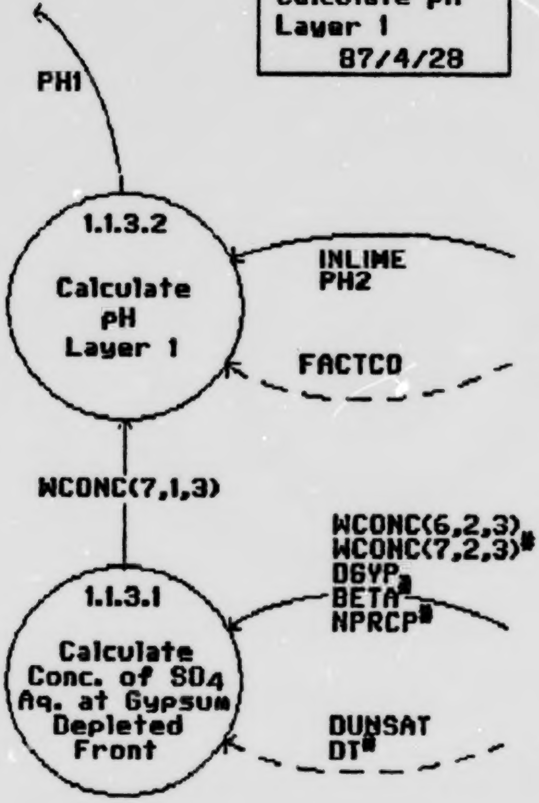
$$[\text{mol m}^{-3}] + ([\text{mol m}^{-3}] - [\text{mol m}^{-3}])\ [-] = [\text{mol m}^{-3}]$$

$$\text{EXP}\ \frac{[\text{m a}^{-1}] * [\text{a}]}{[-] * [\text{m}]} = [-]$$

Note 1: $[SO_4^{2-}]_{p,\lambda w,t} \equiv [SO_4^{2-}]_{p,\lambda w}$

Note 2: The solution concentration of sulphate from pyrite dissolution is assumed to be zero at t=-Δt.

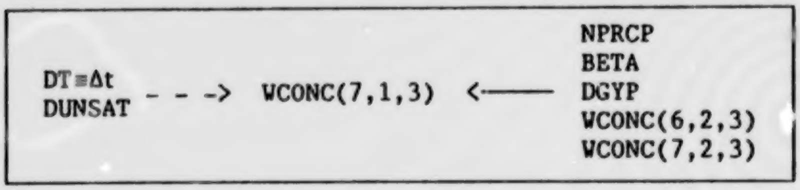
Figure 1.1.3
Calculate pH
Layer 1
87/4/28


PH1
1.1.3.2
Calculate pH Layer 1
INLIME
PH2
FACTCO
WCONC(7,1,3)
WCONC(6,2,3),
WCONC(7,2,3)#
DGYP,
BETA#
NPRCP#
1.1.3.1
Calculate Conc. of SO_4 Aq. at Gypsum Depleted Front
DUNSAT
DT#

Note: variables marked with "#" are not required in the DDD, as deduced from inspection of the UTAP2 code.

Figure 1.1.3.1
Calculate CONC. OF SO_4 AQ. AT GYPSUM-DEPLETED FRONT (WCONC(7,1,3))

WCONC(7,1,3) - CONC. OF SO_4 AQ. AT GYPSUM-DEPLETED FRONT [mol m^{-3}]. Total concentration of sulphate ions in the aqueous phase at the bottom of the gypsum-depleted front of the unsaturated zone (from pyrite oxidation and downward movement of water as a function of time).



Short Name	Long Name	SI Unit	Source
BETA	PYRITE OXIDATION FACTOR	[mol m^{-3}]	1.1.2.4
DGYP	DEPTH OF UPPER UNSAT. ZONE	[m]	1.1.2.6
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled
WCONC(6,2,3)	CONC. OF SO_4 AQ. AT BOTTOM OF UNSAT. ZONE FROM PYRITE	[mol m^{-3}]	1.1.2.10
WCONC(7,1,3)	CONC. OF SO_4 AQ. AT GYPSUM-DEPLETED FRONT	[mol m^{-3}]	1.1.3.1
WCONC(7,2,3)	CONC. OF SO_4 AQ. BOTTOM UNSAT. ZONE	[mol m^{-3}]	1.1.2.11

$$\mathrm{WCONC(7,1,3)} = \frac{2.0 * \mathrm{DGYP} * \mathrm{BETA}}{\mathrm{NPRCP} * \mathrm{DT}} + 0.1$$

(eqn. 3.3.36; see Notes 5 to 7)

Unit check:

$$\frac{[-] * [m] * [mol\ m^{-3}]}{[m\ a^{-1}] * [a]} + [mol\ m^{-3}] = [mol\ m^{-3}]$$

Note 1: The parameter "2" is assumed to be dimensionless.

Note 2: The assumption is made that DGYP ≡ h ≡ h_t ≡ DGYP(3).

Note 3: BETA, defined near equation (3.3.22), is used to simplify the equation.

Note 4: 0.1 [mol m^{-3}] is sulphate from background precipitation (see SENES pg. 3-10).

Note 5: Inspection of the UTAP2 code shows that WCONC(7,1,3)=0 at t=0. (BWG, 87-03-30).

Note 6: Inspection of the UTAP2 code shows that, once gypsum has been depleted from layer 2 (i.e. DGYP $\geq$ DUNSAT), WCONC(7,1,3) = WCONC(7,2,3). (BWG, 87-04-28)

Note 7: Inspection of the UTAP2 code shows that (for t>0) the above equation is not used for WCONC(7,1,3). Instead, when gypsum is not depleted (cf. Note 5), WCONC(7,1,3) = WCONC(6,2,3) * DGYP / DUNSAT. When GYPSUM is depleted (DGYP $\geq$ DUNSAT), this equation reduces to WCONC(7,1,3) = WCONC(6,2,3). This charge has been implemented into SYVAC3-UT2. (BWG, 87-04-28)

PH1 - PH LAYER 1 [-]. The pH of solution in the gypsum-depleted layer of the unsaturated zone of the tailings.

Figure 1.1.3.2
Calculate PH LAYER 1
(PH1)
(Page 1 of 2)

WCONC(7,1,3)
FACTCO - - -> PH1 <—— INLIME
PH2

Short Name	Long Name	SI Unit	Source
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
INLIME	INVENT. $CACO_3$	[mol m^{-3}]	1.1.2.5
PH1	PH LAYER 1	[-]	1.1.3.2
PH2	PH LAYER 2	[-]	1.2.1.8
WCONC(7,1,3)	CONC. OF SO_4 AQ. AT GYPSUM-DEPLETED FRONT	[mol m^{-3}]	1.1.3.1

If t=0 then PH1 = PH2 (see Note 3)

Otherwise pH1 is calculated iteratively using:

(a) If INLIME = 0 then

$$\frac{10^{-PH1}}{(FACTCO)^{0.25}} + 3\left(\frac{10^{6.5}}{(FACTCO)^{2.25}} + 10^{5.97}\right)10^{-3*PH1} + 2\left(\frac{10^{1.53}}{FACTCO} + 10^{3.78}\right)$$

$$* \; 10^{-2*PH1} + 10^{(0.3-PH1)} = \frac{WCONC(7,1,3)}{1000}$$

$$* \left(\frac{2-(FACTCO)^{0.75}*(10^{(9.7-3*PH1)})-(FACTCO)^{3}*(10^{(8.99-3*PH1)})}{1+(FACTCO)^{0.75}*(10^{(9.7-3*PH1)})+(FACTCO)^{3}*(10^{(8.99-3*PH1)})}\right) + \left(\frac{10^{(PH1-11.27)}}{FACTCO^{0.25}}\right)$$

(eqn. 3.6.17;
see Note 4)

(b) If INLIME > 0 then

$$2\left(\frac{10^{(11.87-2*PH1)}}{FACTCO}\right) + 10^{(0.3-PH1)} = \frac{2*WCONC(7,1,3)}{1000} + \frac{10^{(PH1-9.73)}}{(FACTCO)^{0.25}}$$

(eqn. 3.6.48;
see Note 4)

Unit check:
Each separate term in equations (3.6.17) and (3.6.18) is in [mol dm^{-3}] (SENES pages 3-38, 3-39 respectively). PH1 is dimensionless.

Note 1: SENES "pH" is assumed to be equal to SENES "PH(1)" and "PH1" used here.

Note 2: The term $[SO_4^{2-}]_{T,1}$ in equation (3.6.17) is defined as being in [mol L^{-1}] after equation (3.6.12). $[SO_4^{2-}]_{p,h} \equiv [SO_4^{2-}]_1$ (eqn. (3.3.36)) is defined as being in [mol m^{-3}], equal to WCONC(7,1,3) (Appendix A.3). The factor of 1000 [dm^3 m^{-3}] in equation (3.6.18) is used to convert the sulphate concentration $[SO_4^{2-}]_{p,h}$ to [mol m^{-3}]. Because gypsum has been depleted $[SO_4^{2-}]_{p,h}$ = WCONC(7,1,3).

Figure 1.1.3.2
Calculate PH LAYER 1
(PH1)
(Page 2 of 2)

Note 3: The initial condition for PH1 is described in Section 3.2.3 of the SENES report (BWG, 87-04-02).

Note 4: Inspection of the UTAP2 code shows that WCONC(6,1,3) is used instead of WCONC(7,1,3), and the factor $10^{8.97}$ instead of $10^{8.99}$ (both changes occur twice). The factor $10^{8.97}$ is used in SYVAC3-UT2. WCONC(7,1,3) is still used in SYVAC3-UT2, since an examination of the UTAP2 logic shows that WCONC(7,1,3) = WCONC(6,1,3) for all combinations of the gypsum and lime options. (BWG, 87-04-07 and 87-04-29)

Note 5: Inspection of the UTAP2 code shows that, for the lime option, and when gypsum has been depleted (i.e. DGYP $\geq$ DUNSAT)

PH1 = PH2

In DDD 1.1.2.8, Note 7 points out that under the above conditions PH2 = PH1 and PH1 is calculated using the equations given above. Consequently the equations given here for PH1 are correct, but do not parallel the logic flow in UTAP2. See also Note 6. (BWG, 87-04-28)

Note 6: Inspection of the UTAP2 code shows that the following logic is used:

```
if ($t \leq 0$)
     PH1 = PH2
else if (INLIME(0) $\leq$ 0)            [no lime added]
     PH1 is calculated iteratively as the solution to eqn.
     (3.6.17), as modified in Note 4.
else if (DGYP(t) $\geq$ DUNSAT)         [lime added, gypsum depleted]
     PH1 = PH2
else if (INLIME($t-\Delta t$) > 0)      [gypsum remains, lime remains]
     PH1 is calculated iteratively as the solution to eqn.
     (3.6.48).
else                                    [gypsum remains, lime depleted]
     PH1 is calculated iteratively as the solution to eqn.
     (3.6.17), as modified in Note 4.
```

SYVAC3-UT2 has been adapted to use this logic. (THA, 87-04-30)

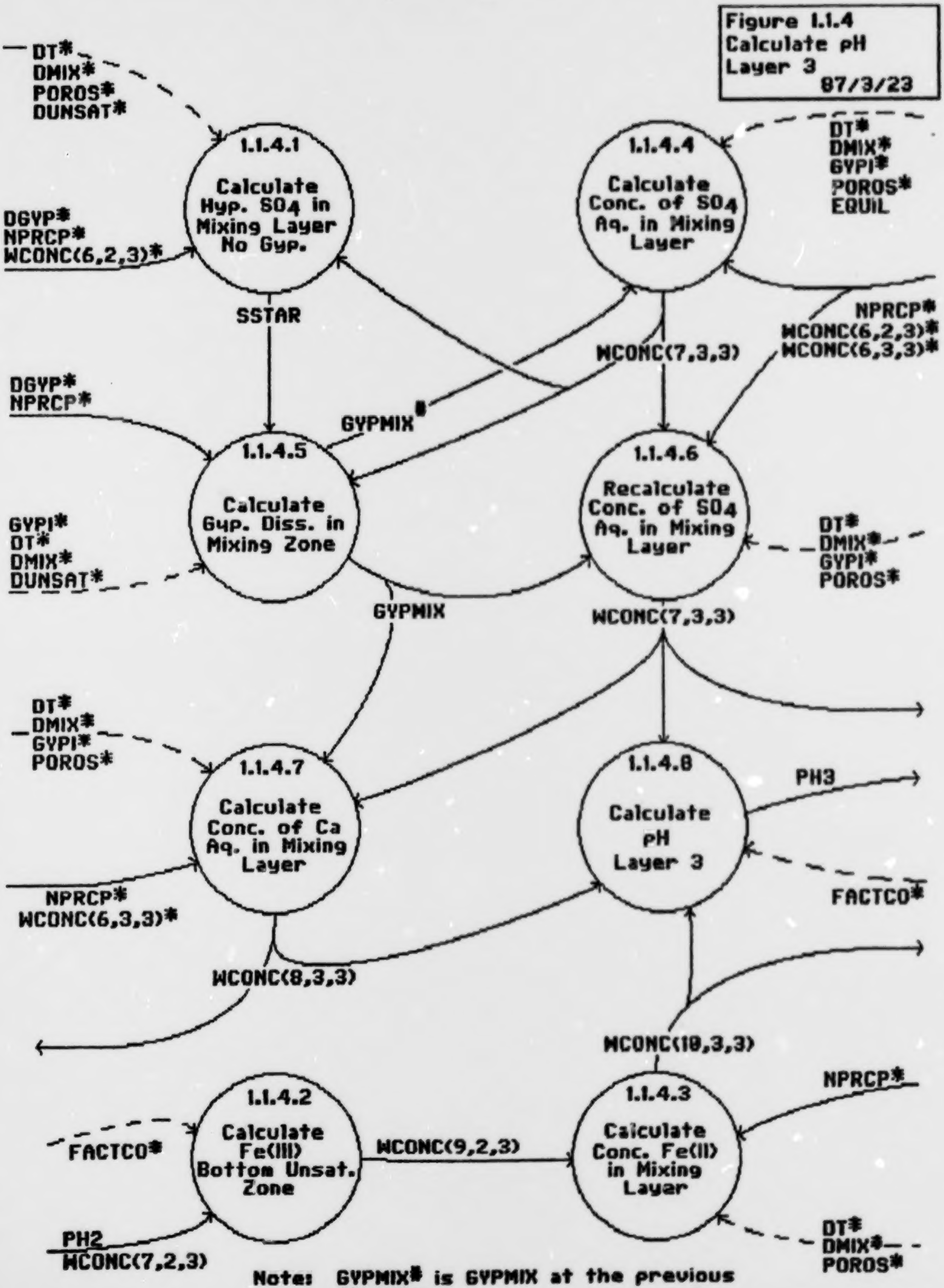


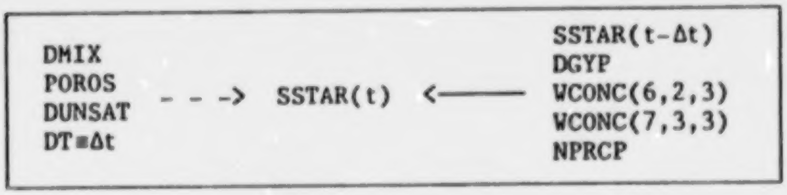
Figure 1.1.4
Calculate pH
Layer 3
87/3/23

DT*
DMIX*
POROS*
DUNSAT*
1.1.4.1
Calculate Hyp. SO4 in Mixing Layer No Gyp.
DGYP*
NPRCP*
WCONC(6,2,3)*
SSTAR
1.1.4.4
Calculate Conc. of SO4 Aq. in Mixing Layer
DT*
DMIX*
GYPI*
POROS*
EQUIL
NPRCP*
WCONC(6,2,3)*
WCONC(6,3,3)*
WCONC(7,3,3)
GYPMIX*
DGYP*
NPRCP*
1.1.4.5
Calculate Gyp. Diss. in Mixing Zone
GYPI*
DT*
DMIX*
DUNSAT*
1.1.4.6
Recalculate Conc. of SO4 Aq. in Mixing Layer
DT*
DMIX*
GYPI*
POROS*
GYPMIX
WCONC(7,3,3)
DT*
DMIX*
GYPI*
POROS*
1.1.4.7
Calculate Conc. of Ca Aq. in Mixing Layer
NPRCP*
WCONC(6,3,3)*
1.1.4.8
Calculate pH Layer 3
PH3
FACTCO*
WCONC(8,3,3)
WCONC(10,3,3)
1.1.4.2
Calculate Fe(III) Bottom Unsat. Zone
FACTCO*
PH2
WCONC(7,2,3)
WCONC(9,2,3)
1.1.4.3
Calculate Conc. Fe(II) in Mixing Layer
NPRCP*
DT*
DMIX*
POROS*

Note: GYPMIX* is GYPMIX at the previous timestep.

Figure 1.1.4.1
Calculate HYP. SO_4 IN
MIXING LAYER NO GYP.
(SSTAR)

SSTAR - HYP. SO_4 IN MIXING LAYER NO GYP. [mol m^{-3}]. Hypothetical concentration of sulphate in the mixing layer if no gypsum were present, calculated for times after gypsum depletion of the unsaturated zone but before gypsum is totally depleted from the mixing layer.



Short Name	Long Name	SI Unit	Source
DGYP	DEPTH OF UPPER UNSAT. ZONE	[m]	1.1.2.6
DMIX	THICKNESS OF MIXING ZONE	[m]	Sampled
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled
POROS	TAILINGS POROSITY	[-]	Sampled
SSTAR	HYP. SO_4 IN MIXING LAYER NO GYP.	[mol m^{-3}]	1.1.4.1
WCONC(6,2,3)	CONC. OF SO_4 AQ. AT BOTTOM OF UNSAT. ZONE FROM PYRITE	[mol m^{-3}]	1.1.2.10
WCONC(7,3,3)	CONC. OF SO_4 AQ. IN MIXING LAYER	[mol m^{-3}]	1.1.4.4

(a) If DGYP < DUNSAT at TIME=t-Δt and DGYP ≥ DUNSAT at TIME=t, then:

$$\text{SSTAR} = \text{WCONC}(7,3,3) \qquad \text{(below eqn. 3.4.8)}$$

(b) If DGYP ≥ DUNSAT at TIME=t-Δt and TIME=t, then:

$$\text{SSTAR}(t) = \text{WCONC}(6,2,3) + \left(\text{SSTAR}(t-\Delta t) - \text{WCONC}(6,2,3)\right) * \text{EXP}\left(\frac{-\text{NPRCP}*\text{DT}}{\text{POROS}*\text{DMIX}}\right) \qquad \text{(eqn. 3.4.8)}$$

(c) SSTAR is not defined for DGYP < DUNSAT at TIME=t

Unit check

(a) SSTAR: [mol m^{-3}] = [mol m^{-3}]

(b) SSTAR: $[\text{mol m}^{-3}] + ([\text{mol m}^{-3}] - [\text{mol m}^{-3}]) * [-] * \text{EXP}\left(\frac{[\text{m a}^{-1}] * [\text{a}]}{[-] * [\text{m}]}\right) = [\text{mol m}^{-3}]$

Note 1: The time the gypsum is depleted from the saturated zone is determined from DGYP < DUNSAT at TIME=t-Δt, but DGYP>DUNSAT at TIME=t.

Note 2: Inspection of the UTAP2 code revealed an error in the DDD; the first condition originally read as (a) If... and DGYP>DUNSAT... Inspection of the UTAP2 code also shows that SSTAR is not changed when GYPMIX(t-Δt) ≥ GYPI. SYVAC3-UT2 was changed accordingly. (BWG, 87-05-12)

WCONC(9,2,3) - CONC. FE(III) AT BOTTOM UNSAT. ZONE [mol m^{-3}]. Concentration of iron(III) in the aqueous phase at the bottom of the unsaturated zone.

Figure 1.1.4.2
Calculate CONC. FE(III)
BOTTOM UNSAT. ZONE
WCONC(9,2,3)

$$\begin{tikzcd} \text{FACTCO} \arrow[r, dashed] & \text{WCONC(9,2,3)} & \begin{array}{l}\text{PH2}\\ \text{WCONC(7,2,3)}\end{array} \arrow[l] \end{tikzcd}$$

Short Name	Long Name	SI Unit	Source
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
PH2	PH LAYER 2	[-]	1.1.2.8
WCONC(7,2,3)	CONC. OF SO_4 AQ. BOTTOM UNSAT. ZONE	[mol m^{-3}]	1.1.2.11
WCONC(9,2,3)	CONC. FE(III) BOTTOM UNSAT. ZONE	[mol m^{-3}]	1.1.4.2

$$\mathrm{WCONC(9,2,3)} = \left\{10^{(5.97-3*\mathrm{PH2})} + 10^{(3.78-2*\mathrm{PH2})} + 10^{(0.3-\mathrm{PH2})}\right.$$

$$\left. + \frac{\mathrm{WCONC(7,2,3)}}{1000} * \left(\frac{\mathrm{FACTCO}^3 * 10^{(8.99-3*\mathrm{PH2})}}{1+\mathrm{FACTCO}^{0.75} * 10^{(9.7-3*\mathrm{PH2})} + \mathrm{FACTCO}^3 * 10^{(8.99-3*\mathrm{PH2})}}\right)\right\} * 1000$$

(eqn. 3.3.44 and below)

Unit check:

$$\left([\mathrm{mol\ dm^{-3}}] + [\mathrm{mol\ dm^{-3}}] + [\mathrm{mol\ dm^{-3}}] + \frac{[\mathrm{mol\ m^{-3}}]}{[\mathrm{dm^3\ m^{-3}}]} * [-]\right) * [\mathrm{dm^3\ m^{-3}}] = [\mathrm{mol\ m^{-3}}]$$

Note 1: Appropriate factors of 1000 [dm^3 m^{-3}] have been used to maintain consistent units of [mol m^{-3}].

Note 2: Assumes pH = pH(2) ≡ pH2.

Note 3: Appendix A.2 has $[\mathrm{Fe(III)}]_{\lambda_w}$ = WCONC(9,2,3), Appendix A.3 has $[\mathrm{Fe}^{3+}]_{\lambda_w}$ = WCONC(9,2,3). Based on the text near equation (3.3.44) the former was assumed correct.

Figure 1.1.4.3
Calculate CONC. FE(II)
IN MIXING LAYER
(WCONC(10,3,3))

WCONC(10,3,3) - CONC. FE(II) IN MIXING LAYER $[\mathrm{mol\ m^{-3}}]$. Concentration of iron(II) in the aqueous phase in the mixing layer of the saturated zone.

```
DT≡Δt                                          WCONC(9,2,3)
POROS   - - ->  WCONC(10,3,3)  <———————        WCONC(10,3,2)
DMIX                                           NPRCP
```

Short Name	Long Name	SI Unit	Source
DMIX	THICKNESS OF MIXING ZONE	[m]	Sampled
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
NPRCP	NET PRECIPITATION	$[\mathrm{m\ a^{-1}}]$	Sampled
POROS	TAILINGS POROSITY	[-]	Sampled
WCONC(9,2,3)	CONC. FE(III) BOTTOM UNSAT. LAYER	$[\mathrm{mol\ m^{-3}}]$	1.1.4.2
WCONC(10,3,2)	CONC. FE(II) IN MIXING LAYER (at TIME= (t-Δt))	$[\mathrm{mol\ m^{-3}}]$	(1.1.4.3)
WCONC(10,3,3)	CONC. FE(II) IN MIXING LAYER (at TIME=t)	$[\mathrm{mol\ m^{-3}}]$	1.1.4.3

For t=0, WCONC(10,3,3) = 1.5 * WCONC(9,2,3) (eqn. 3.2.11; see Note 4)

For t>0,

$$\mathrm{WCONC}(10,3,3) = 1.5 * \mathrm{WCONC}(9,2,3) + (\mathrm{WCONC}(10,3,2) - 1.5 * \mathrm{WCONC}(9,2,3)) * \mathrm{EXP}\left(\frac{-\ \mathrm{NPRCP} * \mathrm{DT}}{\mathrm{POROS} * \mathrm{DMIX}}\right) \quad \text{(eqn. 3.4.16)}$$

Unit check

$$\mathrm{WCONC}(10,3,3){:}\ [\mathrm{mol\ m^{-3}}] + ([\mathrm{mol\ m^{-3}}] - [\mathrm{mol\ m^{-3}}]) * [-] = [\mathrm{mol\ m^{-3}}]$$

$$\mathrm{EXP}{:}\quad \frac{[\mathrm{m\ a^{-1}}] * [\mathrm{a}]}{[-] * [\mathrm{m}]} = [-]$$

Note 1: WCONC(9,2,3) ≡ $[\mathrm{Fe^{III}}]_{\lambda_w}$, WCONC(10,3,3) ≡ $[\mathrm{Fe^{II}}]_{mix,t}$ from Appendix A.2. The definitions in Appendix A.3 are assumed to be in error.

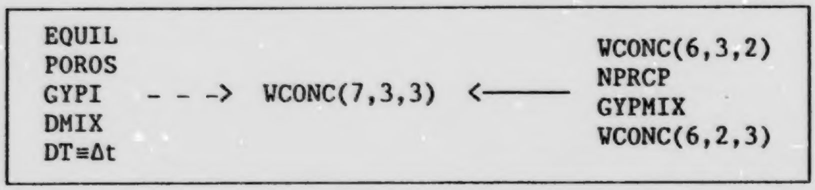
Note 2: WCONC(10,3,2) ≡ WCONC(10,3,1) is assumed equal to zero at time t=-Δt.

Note 3: The factors 1.5 are dimensionless stoichiometry factors.

Note 4: Initial condition deduced following an examination of the UTAP2 code. The original specification used eqn. (3.4.16) for an initial condition.

WCONC(7,3,3) - CONC. OF SO_4 AQ. IN MIXING LAYER [mol m^{-3}]. The total concentration of sulphate ions in the aqueous phase in the mixing layer of the saturated zone.

Figure 1.1.4.4
Calculate CONC. OF SO_4 AQ. IN MIXING LAYER (WCONC(7,3,3))



Short Name	Long Name	SI Unit	Source
DMIX	THICKNESS OF MIXING ZONE	[m]	Sampled
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
EQUIL	SQ. ROOT OF EQBM. CONST. GYPSUM	[mol m^{-3}]	1.1.1.2
GYPI	INIT. GYPSUM CONTENT IN TAILINGS	[mol m^{-3}]	1.1.1.1
GYPMIX	GYP. DISS. IN MIXING ZONE (at TIME=(t-Δt))	[mol m^{-3}]	1.1.4.5
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled
POROS	TAILINGS POROSITY	[-]	Sampled
WCONC(6,2,3)	CONC. OF SO_4 AQ. AT BOTTOM OF UNSAT. ZONE FROM PYRITE	[mol m^{-3}]	1.1.2.10
WCONC(6,3,2)	CONC. OF SO_4 AQ. IN MIXING LAYER FROM PYRITE (at TIME=(t-Δt))	[mol m^{-3}]	1.1.2.13
WCONC(7,3,3)	CONC. OF SO_4 AQ. IN MIXING LAYER	[mol m^{-3}]	1.1.4.4

(a) If GYPMIX(t-Δt) < GYPI (or GYPMIX(t) < GYPI for t=-Δt)

$$\mathrm{WCONC(7,3,3)} = (\mathrm{EQUIL} * \mathrm{EQUIL} + 0.25 * \mathrm{WCONC(6,3,3)} * \mathrm{WCONC(6,3,3)})^{0.5} + 0.5 * \mathrm{WCONC(6,3,3)} \qquad \text{(eqn. 3.4.7)}$$

(b) If GYPMIX (t-Δt) ≥ GYPI

$$\mathrm{WCONC(7,3,3)} = \mathrm{WCONC(6,2,3)} + (\mathrm{WCONC(6,3,2)} - \mathrm{WCONC(6,2,3)}) * \mathrm{EXP}\left(\frac{-\mathrm{NPRCP} * \mathrm{DT}}{\mathrm{POROS} * \mathrm{DMIX}}\right) \qquad \text{(eqn. 3.4.12; see Note 4)}$$

Unit check

(a) $$\left([\mathrm{mol\ m^{-3}}] * [\mathrm{mol\ m^{-3}}] + [\mathrm{mol\ m^{-3}}] * [\mathrm{mol\ m^{-3}}]\right)^{0.5} + [\mathrm{mol\ m^{-3}}] = [\mathrm{mol\ m^{-3}}]$$

(b) $$[\mathrm{mol\ m^{-3}}] + \left([\mathrm{mol\ m^{-3}}] - [\mathrm{mol\ m^{-3}}]\right) * \mathrm{EXP}\ \frac{[\mathrm{m\ a^{-1}}] * [\mathrm{a}]}{[-] * [\mathrm{m}]} = [\mathrm{mol\ m^{-3}}]$$

Note 1: EQUIL (defined near equation (3.3.22)) has been used to modify (simplify) equation (3.4.7).

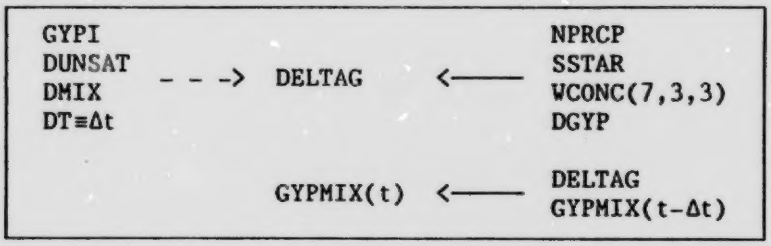
Note 2: 0.25 and 0.5 are assumed dimensionless.

Note 3: The discussion in SENES Vol. 3 pg 3-4 and 3-5 implies that WCONC(7,3,3) = 0 at t=-Δt.

Note 4: Inspection of the UTAP2 code shows that WCONC(7,3,2) is used instead of WCONC(6,3,2) in eqn. (3.4.12). (BWG, 87-05-07)

GYPMIX - GYP. DISS. IN MIXING ZONE [mol m^{-3}].
The total gypsum per unit volume dissolved in the mixing zone to any TIME=t.

Figure 1.1.4.5
Calculate GYP. DISS.
IN MIXING ZONE
(GYPMIX)



Short Name	Long Name	SI Unit	Source
DELTAG	GYP. DISS. IN MIXING ZONE IN TIME INT.	[mol m^{-3}]	(1.1.4.5)
DGYP	DEPTH OF UPPER UNSAT. ZONE	[m]	1.1.2.6
DMIX	THICKNESS OF MIXING ZONE	[m]	Sampled
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
GYPI	INIT. GYPSUM CONTENT IN TAILINGS	[mol m^{-3}]	1.1.1.1
GYPMIX	GYP. DISS. IN MIXING ZONE (at TIME= (t-Δt))	[mol m^{-3}]	1.1.4.5
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled
SSTAR	HYP. SO_4 IN MIXING LAYER NO GYP.	[mol m^{-3}]	1.1.4.1
WCONC(7,3,3)	CONC. OF SO_4 AQ. IN MIXING LAYER	[mol m^{-3}]	1.1.4.4

If DGYP < DUNSAT DELTAG = 0

$$\text{If} \quad \text{DGYP} \geq \text{DUNSAT} \qquad \text{DELTAG} = \frac{\text{NPRCP} * \text{DT}}{\text{DMIX}} * \left(\text{WCONC}(7,3,3)-\text{SSTAR}\right)$$

(eqn. 3.4.9)

From the finite difference equation

$$\text{GYPMIX}(t) = \text{GYPMIX}(t-\Delta t) + \text{DELTAG}$$

(eqn. 3.4.10 modified)

Unit check

$$\text{DELTAG:} \quad \frac{[\text{m a}^{-1}] * [\text{a}]}{[\text{m}]} * \left([\text{mol m}^{-3}] - [\text{mol m}^{-3}]\right) = [\text{mol m}^{-3}]$$

$$\text{GYPMIX:} \quad [\text{mol m}^{-3}] + [\text{mol m}^{-3}] = [\text{mol m}^{-3}]$$

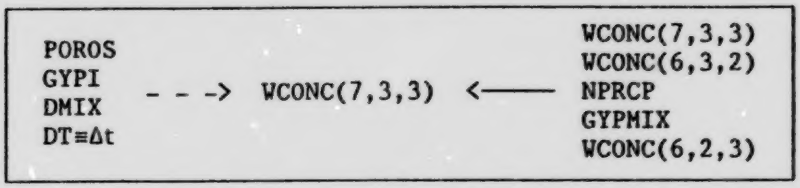
Note 1: The equivalent finite difference equation has been used instead of the summation in equation (3.4.10).

Note 2: GYPMIX = 0 at t=-Δt by definition.

Note 3: Inspection of the UTAP2 code shows that, if GYPMIX(t) ≥ GYPI, DELTAG = 0 and GYPMIX(t) = GYPI. (BWG, 87-05-13)

Figure 1.1.4.6
Recalculate CONC. OF
S04 AQ. IN MIXING
LAYER (WCONC(7,3,3))

WCONC(7,3,3) - CONC. OF S04 AQ. IN MIXING LAYER [mol m-3]. The total concentration of sulphate ions in the aqueous phase in the mixing layer of the saturated zone.



Short Name	Long Name	SI Unit	Source
DMIX	THICKNESS OF MIXING ZONE	[m]	Sampled
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
GYPI	INIT. GYPSUM CONTENT IN TAILINGS	[mol m^{-3}]	1.1.1.1
GYPMIX	GYP. DISS. IN MIXING ZONE (at TIME=t)	[mol m^{-3}]	1.1.4.5
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled
POROS	TAILINGS POROSITY	[m^3 m^{-3}]	Sampled
WCONC(6,2,3)	CONC. OF SO_4 AQ. AT BOTTOM OF UNSAT. ZONE FROM PYRITE	[mol m^{-3}]	1.1.2.10
WCONC(6,3,2)	CONC. OF SO_4 AQ. IN MIXING LAYER FROM PYRITE (at TIME=t-Δt)	[mol m^{-3}]	1.1.2.13
WCONC(7,3,3)	CONC. OF SO_4 AQ. IN MIXING LAYER	[mol m^{-3}]	1.1.4.4 & 1.1.4.6

(a) If GYPMIX (TIME=(t-Δt)) < GYPI and GYPMIX (TIME=t) ≥ GYPI

$$\text{WCONC}(7,3,3) = \text{WCONC}(6,2,3) + (\text{WCONC}(6,3,2) - \text{WCONC}(6,2,3)) * \text{EXP}\left(\frac{-\text{NPRCP} * \text{DT}}{\text{POROS} * \text{DMIX}}\right)$$

(eqn. 3.4.12; see Note 2)

(b) If GYPMIX (TIME=(t-Δt) ≥ GYPI or GYPMIX (TIME=t) < GYPI

$$\text{WCONC}(7,3,3) = \text{WCONC}(7,3,3)$$

Unit check:

$$\text{(a)}\quad [\text{mol m}^{-3}] = [\text{mol m}^{-3}] + ([\text{mol m}^{-3}] - [\text{mol m}^{-3}]) * \text{EXP}\left(\frac{[\text{m a}^{-1}] * [\text{a}]}{[-] * [\text{m}]}\right)$$

$$= [\text{mol m}^{-3}]$$

Note 1: When GYPMIX (TIME=t-Δt) < GYPI and GYPMIX (TIME=t) ≥ GYPI, WCONC(7,3,3) must be calculated twice, once using equation (3.4.7) to establish GYPMIX and once using equation (3.4.12) to get a better value for WCONC(7,3,3). This method conforms to the statement in SENES Vol. 3 pg. 3-28 that equation (3.4.12) should be used if $[gyp]_{diss,t} = g_o$. Thus, WCONC(7,3,3) is calculated in Figure 1.1.4.4, and recalculated in Figure 1.1.4.6 if necessary.

Note 2: Inspection of the UTAP2 code shows that WCONC(7,3,2) is used instead of WCONC(6,3,2) in eqn. (3.4.12). (BWG, 87-05-07)

WCONC(8,3,3) - CONC. OF CA AQ. IN MIXING LAYER [mol m^{-3}]. The concentration of calcium ions in the aqueous phase in the mixing layer of the saturated zone.

Figure 1.1.4.7
Calculate CONC. OF CA AQ. IN MIXING LAYER (WCONC(8,3,3))

DT≡Δt
DMIX
POROS - - -> WCONC(8,3,3) <—— NPRCP
GYPI

WCONC(8,3,2)
WCONC(7,3,3)
NPRCP
WCONC(6,3,3)
GYPMIX

Short Name	Long Name	SI Unit	Source
DMIX	THICKNESS OF MIXING ZONE	[m]	Sampled
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
GYPI	INIT. GYPSUM CONTENT IN TAILINGS	[mol m^{-3}]	1.1.1.1
GYPMIX	GYP. DISS. IN MIXING ZONE	[mol m^{-3}]	1.1.4.5
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled
POROS	TAILINGS POROSITY	[-]	Sampled
WCONC(6,3,3)	CONC. OF SO_4 AQ. IN MIXING LAYER FROM PYRITE	[mol m^{-3}]	1.1.2.13
WCONC(7,3,3)	CONC. OF SO_4 AQ. IN MIXING LAYER	[mol m^{-3}]	1.1.4.6
WCONC(8,3,2)	CONC. OF CA AQ. IN MIXING LAYER (TIME=(t-Δt))	[mol m^{-3}]	(1.1.4.7)
WCONC(8,3,3)	CONC. OF CA AQ. IN MIXING LAYER (TIME=t)	[mol m^{-3}]	1.1.4.7

(a) If GYPMIX < GYPI

$$WCONC(8,3,3) = WCONC(7,3,3) - WCONC(6,3,3)$$ (eqn. 3.4.6 & 3.4.7 see Notes)

(b) If GYPMIX ≥ GYPI from the finite difference equation

$$WCONC(8,3,3) = WCONC(8,3,2) * EXP\left(\frac{-NPRCP * DT}{POROS * DMIX}\right)$$ (eqn. 3.4.11)

Unit check

(a) $[mol\ m^{-3}] - [mol\ m^{-3}] = [mol\ m^{-3}]$

(b) $[mol\ m^{-3}] * [-] = [mol\ m^{-3}]$

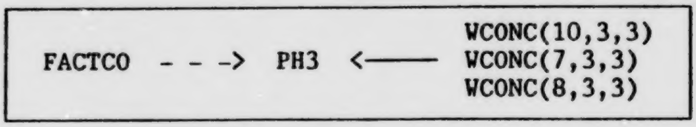
$$EXP: \frac{[m\ a^{-1}] * [a]}{[-] * [m]} = [-]$$

Note 1: Subtraction of equation (3.4.7) from equation (3.4.6) gives the equation used here.

Note 2: Inspection of the UTAP2 code shows that GYPMIX used in comparison (a) is GYPMIX(t-Δt). (BWG, 87-05-12)

PH3 - PH LAYER 3 [-]. The pH of solution in the mixing layer of the saturated zone of the tailings.

Figure 1.1.4.8
Calculate
PH LAYER 3
(PH3)



Short Name	Long Name	SI Unit	Source
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
PH3	PH LAYER 3	[-]	1.1.4.8
WCONC(7,3,3)	CONC. OF SO_4 AQ. IN MIXING LAYER	[mol m^{-3}]	1.1.4.4
WCONC(8,3,3)	CONC. OF CA AQ. IN MIXING LAYER	[mol m^{-3}]	1.1.4.7
WCONC(10,3,3)	CONC. FE(II) IN MIXING LAYER	[mol m^{-3}]	1.1.4.3

Calculated iteratively from

$$2*\frac{\mathrm{WCONC}(8,3,3)}{1000} + 2*\frac{\mathrm{WCONC}(10,3,3)}{1000} + 3*\left(\frac{10^{(6.8-3*\mathrm{PH3})}}{(\mathrm{FACTCO})^{2.25}}\right) + 2*\left(\frac{10^{(1.83-2*\mathrm{PH3})}}{\mathrm{FACTCO}}\right)$$

$$+\frac{10^{3.1-\mathrm{PH3}}}{(\mathrm{FACTCO})^{0.25}} = \frac{\mathrm{WCONC}(7,3,3)}{1000} * \left(\frac{2-(\mathrm{FACTCO})^{0.75} * 10^{(9.7-3*\mathrm{PH3})}}{1+(\mathrm{FACTCO})^{0.75} * 10^{(9.7-3*\mathrm{PH3})}}\right)$$

$$+\frac{10^{(\mathrm{PH3}-10.47)}}{(\mathrm{FACTCO})^{0.25}} \qquad \text{(eqn. 3.6.35)}$$

Unit check for equation

$$\left(\frac{[\mathrm{mol\ m^{-3}}]}{[\mathrm{dm\ m^{-3}}]} + \frac{[\mathrm{mol\ m^{-3}}]}{[\mathrm{dm\ m^{-3}}]} + \mathrm{mol\ dm^{-3}}] + [\mathrm{mol\ dm^{-3}}] + [\mathrm{mol\ dm^{-3}}]\right.$$

$$\left. = \frac{[\mathrm{mol\ m^{-3}}]}{[\mathrm{dm^3\ m^{-3}}]} * [-] + [\mathrm{mol\ dm^{-3}}]\right) = [\mathrm{mol\ dm^{-3}}]$$

pH is dimensionless

Note 1: The factors of 1000 [dm^3 m^{-3}] are required to convert the concentrations of calcium, sulphate and iron(II) to [mol dm^{-3}].

Note 2: It is assumed that pH used here = pH_{mix} = pH(3) = PH3.

Note 3: Numerical factors 2 and 3 are assumed to be dimensionless.

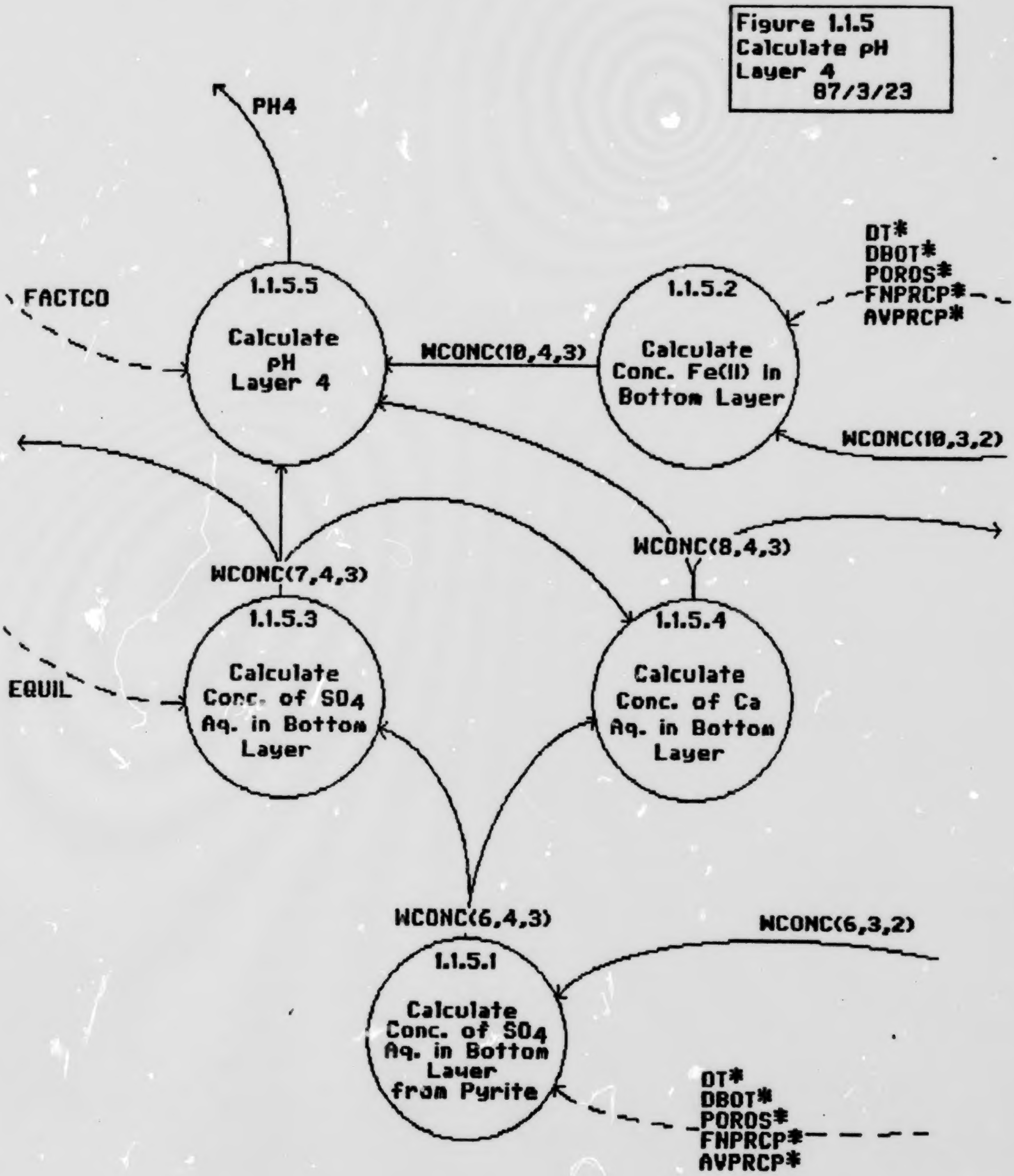
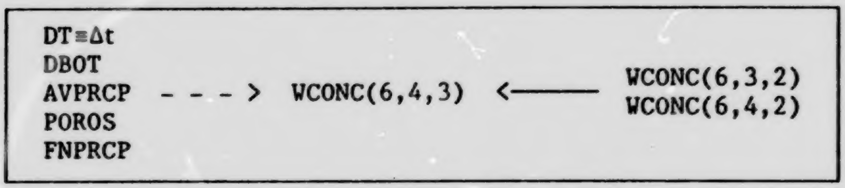


Figure 1.1.5
Calculate pH
Layer 4
87/3/23
PH4
FACTCO
1.1.5.5
Calculate
pH
Layer 4
WCONC(10,4,3)
1.1.5.2
Calculate
Conc. Fe(II) in
Bottom Layer
DT*
DBOT*
POROS*
FNPRCP*
AVPRCP*
WCONC(10,3,2)
WCONC(8,4,3)
WCONC(7,4,3)
1.1.5.3
Calculate
Conc. of SO4
Aq. in Bottom
Layer
EQUIL
1.1.5.4
Calculate
Conc. of Ca
Aq. in Bottom
Layer
WCONC(6,4,3)
WCONC(6,3,2)
1.1.5.1
Calculate
Conc. of SO4
Aq. in Bottom
Layer
from Pyrite
DT*
DBOT*
POROS*
FNPRCP*
AVPRCP*

WCONC(6,4,3) - CONC. OF SO_4 AQ. IN BOTTOM LAYER FROM PYRITE [mol m^{-3}]. Concentration of sulphate ions in the aqueous phase in the bottom layer of the saturated zone, due to pyrite oxidation and downward movement of water (including sulphate in precipitation) as a function of time.

Figure 1.1.5.1
Calculate CONC. OF SO_4 AQ IN BOTTOM LAYER FROM PYRITE (WCONC(6,4,3))



Short Name	Long Name	SI Unit	Source
AVPRCP	AVERAGE NET PRECIPITATION	[m a^{-1}]	Sampled
DBOT	THICKNESS LAYER 4	[m]	1.1.1.4
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
FNPRCP	FRACT. NET PRECIP.	[-]	Sampled
POROS	TAILINGS POROSITY	[-]	Sampled
WCONC(6,3,2)	CONC. OF SO_4 AQ IN MIXING LAYER FROM PYRITE (at TIME=(t-Δt))	[mol m^{-3}]	1.1.2.13
WCONC(6,4,2)	CONC. OF SO_4 AQ IN BOTTOM LAYER FROM PYRITE (at TIME=(t-Δt))	[mol m^{-3}]	(1.1.5.1)
WCONC(6,4,3)	CONC. OF SO_4 AQ IN BOTTOM LAYER FROM PYRITE (at TIME=t)	[mol m^{-3}]	1.1.5.1

Calculated from the finite difference equation

$$\text{WCONC}(6,4,3) = \text{WCONC}(6,3,2) + (\text{WCONC}(6,4,2) - \text{WCONC}(6,3,2)) * \text{EXP}\left(-\frac{\text{FNPRCP*AVPRCP*DT}}{\text{POROS*DBOT}}\right) \qquad \text{(eqn. 3.5.2)}$$

Unit check

WCONC(6,4,3): [mol m^{-3}] + ([mol m^{-3}] - [mol m^{-3}]) [-] = [mol m^{-3}]

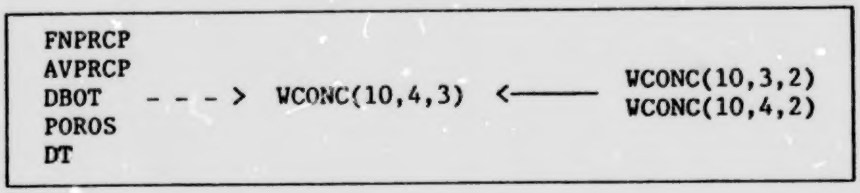
$$\text{EXP:} \quad \frac{[-] * [m\ a^{-1}] * [a]}{[-] * [m]} = [-]$$

Note 1: WCONC(6,4,3) = 0 at t=0 (eqn 3.2.5) (although this does not allow for the 0.1 [mol m^{-3}] background value) and SENES seems to have decided to leave this initial condition stand).

Note 2: WCONC(6,4,2) = 0 (or actually is undefined) for t=0.

Figure 1.1.5.2
Calculate CONC. FE(II)
IN BOTTOM LAYER
(WCONC(10,4,3))

WCONC(10,4,3) - CONC. FE(II) IN BOTTOM LAYER [mol m^{-3}]. Concentration of iron(II) in the aqueous phase in the bottom layer of the saturated zone.



Short Name	Long Name	SI Unit	Source
AVPRCP	AVERAGE NET PRECIPITATION	[m a^{-1}]	Sampled
DBOT	THICKNESS LAYER 4	[m]	1.1.1.4
DT	TIME STEP-SIZE	[a]	Sampled
FNPRCP	FRACT. NET PRECIP.	[-]	Sampled
POROS	TAILINGS POROSITY	[-]	Sampled
WCONC(10,3,2)	CONC. FE(II) IN MIXING LAYER (at TIME=(t-Δt))	[mol m^{-3}]	1.1.4.3
WCONC(10,4,2)	CONC. FE(II) IN BOTTOM LAYER (at TIME=(t-Δt))	[mol m^{-3}]	(1.1.5.2)
WCONC(10,4,3)	CONC. FE(II) IN BOTTOM LAYER (at TIME=t)	[mol m^{-3}]	1.1.5.2

(a) For t>0, calculated from the finite difference equation

$$\text{WCONC(10,4,3)} = \text{WCONC(10,3,2)} + (\text{WCONC(10,4,2)} - \text{WCONC(10,3,2)}) * \text{EXP}\left[- \frac{\text{FNPRCP} * \text{AVPRCP} * \text{DT}}{\text{POROS} * \text{DBOT}}\right] \qquad \text{(eqn. 3.5.5)}$$

(b) For $t \leq 0$, WCONC(10,4,3) = WCONC(10,4,2) = 0 (eqn. 3.2.12)

Unit check:

$$\text{WCONC(10,4,3)}: [\text{mol m}^{-3}] + ([\text{mol m}^{-3}] - [\text{mol m}^{-3}]) * [-] = [\text{mol m}^{-3}]$$

$$\text{EXP:} \frac{[-] * [\text{m a}^{-1}] * [\text{a}]}{[-] * [\text{m}]} = [-]$$

Note: The bold RH bracket in SENES equation (3.5.5) should be before the "exp" (SENES letter (1986-12-09)).

Figure 1.1.5.3
Calculate CONC. OF SO4
AQ. IN BOTTOM LAYER
(WCONC(7,4,3))

WCONC(7,4,3) - CONC. OF SO_4 AQ. IN BOTTOM LAYER [mol m^{-3}]. The total concentration of sulphate ions in the aqueous phase in the bottom layer of the saturated zone.

EQUIL - - - > WCONC(7,4,3) <——— WCONC(6,4,3)

Short Name	Long Name	SI Unit	Source
EQUIL	SQ. ROOT OF EQBM. CONST. GYPSUM	[mol m^{-3}]	1.1.1.2
WCONC(6,4,3)	CONC. OF SO_4 AQ. IN BOTTOM LAYER FROM PYRITE	[mol m^{-3}]	1.1.5.1
WCONC(7,4,3)	CONC. OF SO_4 AQ. IN BOTTOM LAYER	[mol m^{-3}]	1.1.5.3

$$\mathrm{WCONC}(7,4,3) = (\mathrm{EQUIL} * \mathrm{EQUIL} + 0.25 * \mathrm{WCONC}(6,4,3) * \mathrm{WCONC}(6,4,3))^{0.5} + 0.5 * \mathrm{WCONC}(6,4,3) \qquad \text{(eqn. 3.5.4)}$$

Unit check:

$$\mathrm{WCONC}(7,4,3)\text{:}\ \left([\mathrm{mol\ m^{-3}}] * [\mathrm{mol\ m^{-3}}] + [\mathrm{mol\ m^{-3}}] * [\mathrm{mol\ m^{-3}}]\right)^{0.5} + [\mathrm{mol\ m^{-3}}]$$

$$= [\mathrm{mol\ m^{-3}}]$$

Note 1: 0.5 and 0.25 are assumed dimensionless.

Note 2: EQUIL defined near eqn (3.3.22) has been used to modify (simplify) equation (3.5.4).

Figure 1.1.5.4
Calculate CONC. OF CA AQ. IN BOTTOM LAYER (WCONC(8,4,3))

WCONC(8,4,3) - CONC. OF CA AQ. IN BOTTOM LAYER [mol m^{-3}]. Concentration of calcium ions in the aqueous phase in the bottom layer of the saturated zone.

WCONC(8,4,3) <——— WCONC(7,4,3)
WCONC(6,4,3)

Short Name	Long Name	SI Unit	Source
WCONC(6,4,3)	CONC. OF SO_4 AQ. IN BOTTOM LAYER FROM PYRITE	[mol m^{-3}]	1.1.5.1
WCONC(7,4,3)	CONC. OF SO_4 AQ. IN BOTTOM LAYER	[mol m^{-3}]	1.1.5.3
WCONC(8,4,3)	CONC. OF CA AQ. IN BOTTOM LAYER	[mol m^{-3}]	1.1.5.4

WCONC(8,4,3) = WCONC(7,4,3) - WCONC(6,4,3) (eqns. 3.5.3 & 3.5.4)

Unit check:

WCONC(8,4,3): [mol m^{-3}] - [mol m^{-3}] = [mol m^{-3}]

Note: The equation for WCONC(8,4,3) was obtained by subtracting equation (3.5.4) from equation (3.5.3).

PH4 - PH LAYER 4 [-]. The pH of solution in the bottom layer of the saturated zone of the tailings.

Figure 1.1.5.5
Calculate PH LAYER 4

(PH4)

$$\begin{tikzcd}
\text{FACTCO} \arrow[r, dashed] & \text{PH4} & \begin{array}{l}\text{WCONC(8,4,3)}\\ \text{WCONC(7,4,3)}\\ \text{WCONC(10,4,3)}\end{array} \arrow[l]
\end{tikzcd}$$

Short Name	Long Name	SI Unit	Source
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
PH4	PH LAYER 4	[-]	1.1.5.5
WCONC(7,4,3)	CONC. OF SO_4 AQ. IN BOTTOM LAYER	[mol m^{-3}]	1.1.5.3
WCONC(8,4,3)	CONC. OF CA AQ. IN BOTTOM LAYER	[mol m^{-3}]	1.1.5.4
WCONC(10,4,3)	CONC. FE(II) IN BOTTOM LAYER	[mol m^{-3}]	1.1.5.2

Calculated iteratively from

$$\frac{2*\mathrm{WCONC}(8,4,3)}{1000} + \frac{2*\mathrm{WCONC}(10,4,3)}{1000} + 3*\left(\frac{10^{(6.8-3*\mathrm{PH4})}}{(\mathrm{FACTCO})^{2.25}}\right) + 2*\left(\frac{10^{(1.83-2*\mathrm{PH4})}}{\mathrm{FACTCO}}\right)$$
$$+ \frac{10^{(3.1-\mathrm{PH4})}}{(\mathrm{FACTCO})^{0.25}} = \frac{\mathrm{WCONC}(7,4,3)}{1000} * \left(\frac{2-(\mathrm{FACTCO})^{0.75}*10^{(9.7-3*\mathrm{PH4})}}{1+(\mathrm{FACTCO})^{0.75}*10^{(9.7-3*\mathrm{PH4})}}\right)$$
$$+ \frac{10^{(\mathrm{PH4}-10.47)}}{(\mathrm{FACTCO})^{0.25}} \qquad \text{(as in eqn. 3.6.35)}$$

Unit check for eqn

$$\left(\frac{[\mathrm{mol\ m^{-3}}]}{[\mathrm{dm^3\ m^{-3}}]} + \frac{[\mathrm{mol\ m^{-3}}]}{[\mathrm{dm^3\ m^{-3}}]} + [\mathrm{mol\ dm^{-3}}] + [\mathrm{mol\ dm^{-3}}] + [\mathrm{mol\ dm^{-3}}] = \frac{[\mathrm{mol\ m^{-3}}]}{[\mathrm{dm^3\ m^{-3}}]} + [\mathrm{mol\ dm^{-3}}]\right) = [\mathrm{mol\ dm^{-3}}]$$

pH is dimensionless

Note 1: The factors of 1000 [dm^3 m^{-3}] are required to convert the concentrations of calcium, sulphate and iron(II) to [mol dm^{-3}].

Note 2: The equation is (3.6.35) with the modifications given in SENES Vol. 3, Section 3.6.4.

Figure 1.2
Calculate Uranium
Source Concentrations
87/3/27

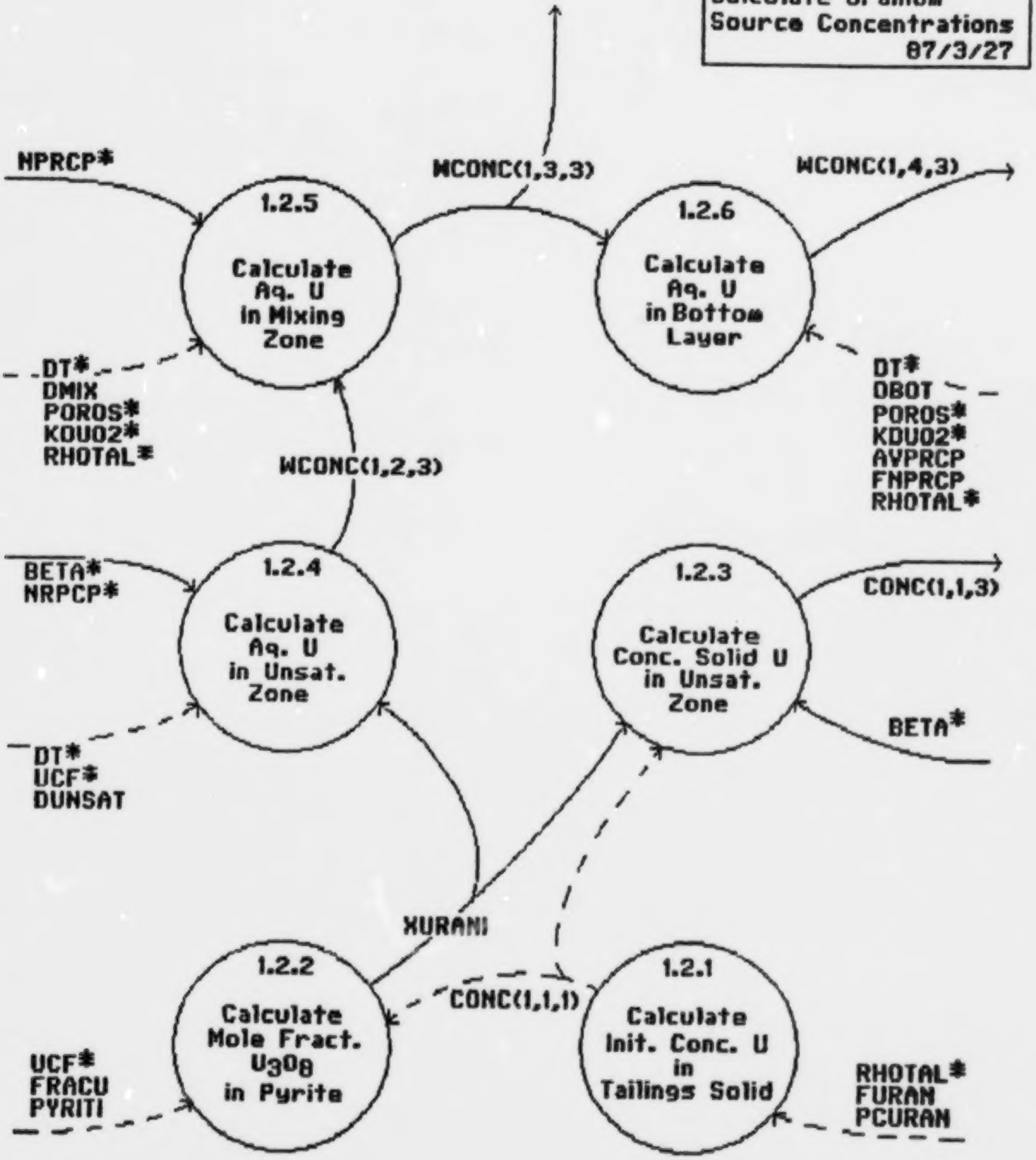

NPRCP*
WCONC(1,3,3)
WCONC(1,4,3)
1.2.5
Calculate
Aq. U
in Mixing
Zone
1.2.6
Calculate
Aq. U
in Bottom
Layer
DT*
DMIX
POROS*
KDUO2*
RHOTAL*
DT*
DBOT
POROS*
KDUO2*
AVPRCP
FNPRCP
RHOTAL*
WCONC(1,2,3)
BETA*
NRPCP*
1.2.4
Calculate
Aq. U
in Unsat.
Zone
1.2.3
Calculate
Conc. Solid U
in Unsat.
Zone
CONC(1,1,3)
BETA*
DT*
UCF*
DUNSAT
XURANI
1.2.2
Calculate
Mole Fract.
U_3O_8
in Pyrite
CONC(1,1,1)
1.2.1
Calculate
Init. Conc. U
in
Tailings Solid
UCF*
FRACU
PYRITI
RHOTAL*
FURAN
PCURAN

Figure 1.2.1
Calculate INIT. CONC.
U IN TAILINGS SOLID
(CONC(1,1,1))

CONC(1,1,1) - INIT. CONC. U IN TAILINGS SOLID [Bq m^{-3}]. Initial concentration of natural uranium in the solid phase of the tailings.

```
RHOTAL
AUNATT    - - ->   CONC(1,1,1)

AUNATO
FURAN     - - ->   AUNATT

PCURAN    - - ->   AUNATO
```

Short Name	Long Name	SI Unit	Source
AUNATO	INITIAL ACTIVITY OF U-NAT IN ORE	[Bq g^{-1}]	(1.2.1)
AUNATT	INITIAL ACTIVITY OF U-NAT IN TAILINGS	[Bq g^{-1}]	(1.2.1)
CONC(1,1,1)	INIT. CONC. U IN TAILINGS SOLID	[Bq m^{-3}]	1.2.1
FURAN	MASS FRACT. U RECOVERED	[-]	Sampled
PCURAN	MASS % U (AS U_3O_8) IN ORE	[-]	Sampled
RHOTAL	TAILINGS BULK DENSITY	[g m^{-3}]	Sampled

$$\text{AUNATO} = \left(\frac{\text{PCURAN}}{100}\right) * \left(\frac{714}{842}\right) * 2.5 * 10^4 \qquad \text{(eqn. 3.7.1)}$$

$$\text{AUNATT} = \text{AUNATO (1-FURAN)} \qquad \text{(eqn. 3.7.3)}$$

$$\text{CONC(1,1,1)} = \text{AUNATT} * \text{RHOTAL} \qquad \text{(eqn. 3.7.4)}$$

Unit check:
AUNATO: $[-] * [g\ g^{-1}] * [Bq\ g^{-1}] = [Bq\ g^{-1}]$
AUNATT: $[Bq\ g^{-1}] * ([-] - [-]) = [Bq\ g^{-1}]$
CONC(1,1,1): $[Bq\ g^{-1}] * [g\ m^{-3}] = [Bq\ m^{-3}]$

Note: The "1" in equation (3.7.3) is assumed to be dimensionless. Units for "714" and "842" are from SENES page 3-53.

Figure 1.2.2
Calculate MOL. FRACT.
U_3O_8 IN PYRITE
(XURANI)

XURANI – MOL. FRACT. U308 IN PYRITE [-]. The fraction (on a molar basis) of U_3O_8 in the initial pyrite component of the tailings.

UPYRI
PYRITI — — –> XURANI

FRACU
UCF — — –> UPYRI
CONC(1,1,1)

Short Name	Long Name	SI Unit	Source
CONC(1,1,1)	INIT. CONC. U IN TAILINGS SOLID	[Bq m^{-3}]	1.2.1
FRACU	FRACT. U_3O_8 ASSOC. WITH PYRITE	[-]	Sampled
PYRITI	INIT. CONC. OF PYRITE IN TAILINGS	[mol m^{-3}]	Sampled
UCF	CONVERSION FACTOR MOL TO BQ (NAT-U)	[Bq mol^{-1}]	Sampled
UPYRI	INIT. CONC. U_3O_8 ASSOC. WITH PYRITE	[mol m^{-3}]	(1.2.2)
XURANI	MOL. FRACT. U_3O_8 IN PYRITE	[-]	1.2.2

$$\mathrm{UPYRI} = \frac{\mathrm{CONC(1,1,1)} * \mathrm{FRACU}}{3 * \mathrm{UCF}} \qquad \text{(eqn. 3.7.6)}$$

$$\mathrm{XURANI} = \mathrm{UPYRI/PYRITI} \qquad \text{(eqn. 3.7.7)}$$

Unit check:

UPYRI $[\mathrm{Bq\ m^{-3}}] * [-] / [\mathrm{Bq\ mol^{-1}}] = [\mathrm{mol\ m^{-3}}]$

XURANI $[\mathrm{mol\ m^{-3}}] / [\mathrm{mol\ m^{-3}}] = [-]$

Note: The "3" in equation 3.7.6 allows for the stoichiometry of U_3O_8 and is dimensionless.

CONC(1,1,3) - CONC. SOLID U IN UNSAT. ZONE [Bq m^{-3}]. Solid phase concentration of uranium in the unsaturated zone.

Figure 1.2.3
Calculate CONC. SOLID U IN UNSAT. ZONE (CONC(1,1,3))

CONC(1,1,1)
XURANI - - -> CONC(1,1,3) <—— CONC(1,1,2)
UCF
BETA

Short Name	Long Name	SI Unit	Source
BETA	PYRITE OXIDATION FACTOR	[mol m^{-3}]	1.1.2.4
CONC(1,1,1)	INIT. CONC. U IN TAILINGS SOLID	[Bq m^{-3}]	1.2.1
CONC(1,1,2)	CONC. SOLID U IN UNSAT. ZONE (at TIME=(t-Δt))	[Bq m^{-3}]	1.2.3
CONC(1,1,3)	CONC. SOLID U IN UNSAT. ZONE (at TIME=t)	[Bq m^{-3}]	1.2.3
UCF	CONVERSION FACTOR MOL TO BQ (NAT-U)	[Bq mol^{-1}]	Sampled
XURANI	MOLE FRACT. U_3O_8 IN PYRITE	[-]	1.2.2

from the finite difference equation

t>0

CONC(1,1,3) = CONC(1,1,2) - 3 * BETA * XURANI * UCF
(eqns. 3.8.2 & 3.8.3)

t=0

CONC(1,1,3) = CONC(1,1,1) - 3 * BETA * XURANI * UCF
(eqns. 3.8.2 & 3.8.3; see note 4)

Unit check:

$$[Bq\ m^{-3}] - [-] * [mol\ m^{-3}] * [-] * [Bq\ mol^{-1}] = [Bq\ m^{-3}]$$

Note 1: In Table A.3 (pg. 12) the units for CONC(1,1,2) and CON(1,1,3) are given as [Bq m^{-3}] but on pg. 3-66, 3-67 as [mol m^{-3}], i.e., differing by a factor of UCF. The factor UCF is used above to keep the units in [Bq m^{-3}].

Note 2: The equation used was obtained by substitution of equation (3.8.2) into equation (3.8.3).

Note 3: BETA (defined near SENES equation (3.3.23)) was used to modify (simplify) equation (3.8.2).

Note 4: Inspection of the UTAP2 code shows that their initial condition is CONC(1,1,3) = CONC(1,1,1) at t=0. This condition is used in SYVAC3-UT2. (BWG, 87-04-02)

WCONC(1,2,3) - AQ. U IN UNSAT. ZONE [Bq m^{-3}]. The concentration of uranium in the aqueous phase at the bottom of the unsaturated zone.

Figure 1.2.4
Calculate AQ. U IN UNSAT. ZONE (WCONC(1,2,3))

DUNSAT
UCF
XURANI - - -> WCONC(1,2,3) <—— BETA
DT≡Δt NPRCP

Short Name	Long Name	SI Unit	Source
BETA	PYRITE OXIDATION FACTOR	[mol m^{-3}]	1.1.2.4
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled
UCF	CONVERSION FACTOR MOL TO BQ (NAT-U)	[Bq mol^{-1}]	Sampled
WCONC(1,2,3)	AQ. U IN UNSAT. ZONE	[Bq m^{-3}]	1.2.4
XURANI	MOL. FRACT. U_3O_8 IN PYRITE	[-]	1.2.2

for $t \geq 0$

$$\text{WCONC}(1,2,3) = \frac{3 * \text{DUNSAT} * \text{XURANI} * \text{BETA} * \text{UCF}}{\text{NPRCP} * \text{DT}} \quad \begin{array}{l}(\text{eqn. } 3.7.8\ t=0)\\(\text{eqn. } 3.8.2\ t>0)\end{array}$$

Unit check:

$$\frac{[\text{m}] * [-] * [\text{mol m}^{-3}] * [\text{Bq mol}^{-1}]}{[\text{m a}^{-1}] * [\text{a}]} = [\text{Bq m}^{-3}]$$

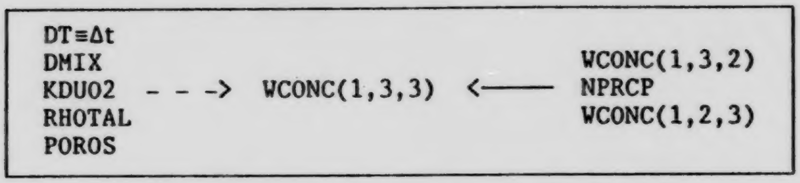
Note 1: Equation (3.8.2) lacks the factor UCF required to convert the concentration from [mol m^{-3}] to [Bq m^{-3}]. The factor has been included here (as it is in equation (3.7.8) for t=0).

Note 2: The factor "3" allows for the stoichiometry of U_3O_8.

Note 3: BETA (defined near SENES equation (3.3.23)) has been substituted in equations (3.7.8) and (3.8.2) to modify (simplify) these equations. In equation (3.7.8), BETA is BETA at t=0.

WCONC(1,3,3) - AQ. U IN MIXING ZONE [Bq m^{-3}]. The concentration of uranium in the aqueous phase in the mixing zone.

Figure 1.2.5
Calculate AQ. U IN MIXING ZONE (WCONC(1,3,3))



Short Name	Long Name	SI Unit	Source
DMIX	THICKNESS OF MIXING ZONE	[m]	Sampled
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
KDUO2	U SOLID-LIQUID DISTR. COEFF.	[m^3 g^{-1}]	Sampled
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled
POROS	TAILINS POROSITY	[m^3 m^{-3}]	Sampled
RHOTAL	TAILINGS BULK DENSITY	[g m^{-3}]	Sampled
WCONC(1,2,3)	AQ. U IN UNSAT. ZONE (at TIME=t)	[Bq m^{-3}]	1.2.4
WCONC(1,3,2)	AQ. U IN MIXING ZONE (at TIME=(t-Δt))	[Bq m^{-3}]	1.2.5
WCONC(1,3,3)	AQ. U IN MIXING ZONE (at TIME=t)	[Bq m^{-3}]	1.2.5

(a) $t > 0$

WCONC(1,3,3) is calculated using the finite difference equation

$$\mathrm{WCONC(1,3,3)} = \mathrm{WCONC(1,2,3)} + \left\{\mathrm{WCONC(1,3,2)} - \mathrm{WCONC(1,2,3)}\right\} * \mathrm{EXP}\left[\frac{-\ \mathrm{NPRCP} * \mathrm{DT}}{\mathrm{POROS} * \mathrm{DMIX} * \left(1 + \dfrac{\mathrm{KDUO2} * \mathrm{RHOTAL}}{\mathrm{POROS}}\right)}\right]$$

(eqn. 3.8.4)

(b) $t = 0$

$$\mathrm{WCONC(1,3,3)} = \mathrm{WCONC(1,2,3)} * \left(1 - \mathrm{EXP}\left[\frac{-\ \mathrm{NPRCP} * \mathrm{DT}}{\mathrm{POROS} * \mathrm{DMIX} * \left(1 + \dfrac{\mathrm{KDUO2} * \mathrm{RHOTAL}}{\mathrm{POROS}}\right)}\right]\right)$$

(eqn. 3.7.9)

Unit check:

(a) WCONC(1,3,3): $[\mathrm{Bq\ m^{-3}}] + \left\{[\mathrm{Bq\ m^{-3}}] - [\mathrm{Bq\ m^{-3}}]\right\} * [-] = [\mathrm{Bq\ m^{-3}}]$

$$\mathrm{EXP:}\ \frac{[\mathrm{m\ a^{-1}}] * [\mathrm{a}]}{[-] * [\mathrm{m}]} \Big/ \left([-] + \frac{[\mathrm{m^3\ g^{-1}}] * [\mathrm{g\ m^{-3}}]}{[-]}\right) = [-]$$

(b) WCONC(1,3,3): $[\mathrm{Bq\ m^{-3}}] * [-] = [\mathrm{Bq\ m^{-3}}]$

EXP: as above

Note: The units of WCONC(1,3,3) are set by those specified for WCONC(1,2,3) and hence do not agree with those noted for equation (3.8.4) in SENES Vol. 3.

SENES keeps the units in [mol m^{-3}] until the last step and then converts to [Bq m^{-3}] but uses the same symbols for the concentrations regardless of units.

Figure 1.2.6
Calculate AQ. U IN
BOTTOM LAYER
(WCONC(1,4,3))

WCONC(1,4,3) - AQ. U IN BOTTOM LAYER [Bq m^{-3}]. The concentration of uranium in the aqueous phase in the bottom layer of the tailings.

$$\begin{tikzcd} \begin{array}{l} \text{AVPRCP} \\ \text{FNPRCP} \\ \text{DBOT} \\ \text{DT} \equiv \Delta t \\ \text{KDUO2} \\ \text{RHOTAL} \\ \text{POROS} \end{array} \arrow[r, dashed] & \text{WCONC(1,4,3)} & \begin{array}{l} \text{WCONC(1,4,2)} \\ \text{WCONC(1,3,3)} \end{array} \arrow[l] \end{tikzcd}$$

Short Name	Long Name	SI Unit	Source
AVPRCP	AVERAGE NET PRECIPITATION	[m a^{-1}]	Sampled
DBOT	THICKNESS LAYER 4	[m]	1.1.1.4
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
FNPRCP	FRACT. NET PRECIP.	[-]	Sampled
KDUO2	U SOLID-LIQUID DISTR. COEFF.	[m^3 g^{-1}]	Sampled
POROS	TAILINGS POROSITY	[m^3 m^{-3}]	Sampled
RHOTAL	TAILINGS BULK DENSITY	[g m^{-3}]	Sampled
WCONC(1,3,3)	AQ. U IN MIXING ZONE (at TIME=t)	[Bq m^{-3}]	1.2.5
WCONC(1,4,2)	AQ. U IN BOTTOM LAYER (at TIME=(t-Δt))	[Bq m^{-3}]	1.2.6
WCONC(1,4,3)	AQ. U IN BOTTOM LAYER (at TIME=t)	[Bq m^{-3}]	1.2.6

(a) $t > 0$

WCONC(1,4,3) is calculated using the finite difference equation

$$\text{WCONC(1,4,3)} = \text{WCONC(1,3,3)} + \{\text{WCONC(1,4,2)} - \text{WCONC(1,3,3)}\} * \text{EXP}\left[\frac{-\text{FNPRCP} * \text{AVPRCP} * \text{DT}}{\text{POROS} * \text{DBOT}} \Big/ \left(1 + \frac{\text{KDUO2} * \text{RHOTAL}}{\text{POROS}}\right)\right] \quad \text{(eqn. 3.8.5)}$$

(b) $t = 0$

$$\text{WCONC(1,4,3)} = \text{WCONC(1,3,3)} * \left(1 - \text{EXP}\left[\frac{-\text{FNPRCP} * \text{AVPRCP} * \text{DT}}{\text{POROS} * \text{DBOT}} \Big/ \left(1 + \frac{\text{KDUO2} * \text{RHOTAL}}{\text{POROS}}\right)\right]\right) \quad \text{(eqn. 3.7.10)}$$

Unit check:

(a) WCONC(1,4,3): [Bq m^{-3}] + {[Bq m^{-3}] - [Bq m^{-3}]} [-]

$$\text{EXP: } \frac{[-] * [\text{m a}^{-1}] * [\text{a}]}{[-] * [\text{m}]} \Big/ \left([-] + \frac{[\text{m}^3\ \text{g}^{-1}] * [\text{g m}^{-3}]}{[-]}\right) = [-]$$

(b) WCONC(1,4,3): [Bq m^{-3}] * [-] = [Bq m^{-3}]

EXP: as above

Note: The units of WCONC(1,4,3) are set by those specified for WCONC(1,3,3) and indirectly WCONC(1,2,3), and hence do not agree with those noted for equation (3.8.5) in SENES Vol. 3. SENES keeps the units in [mol m^{-3}] until the last step and then converts to [Bq m^{-3}] but uses the same symbols for the concentrations, regardless of units.

Figure 1.3
Calculate Thorium
Source Concentrations
87/3/27

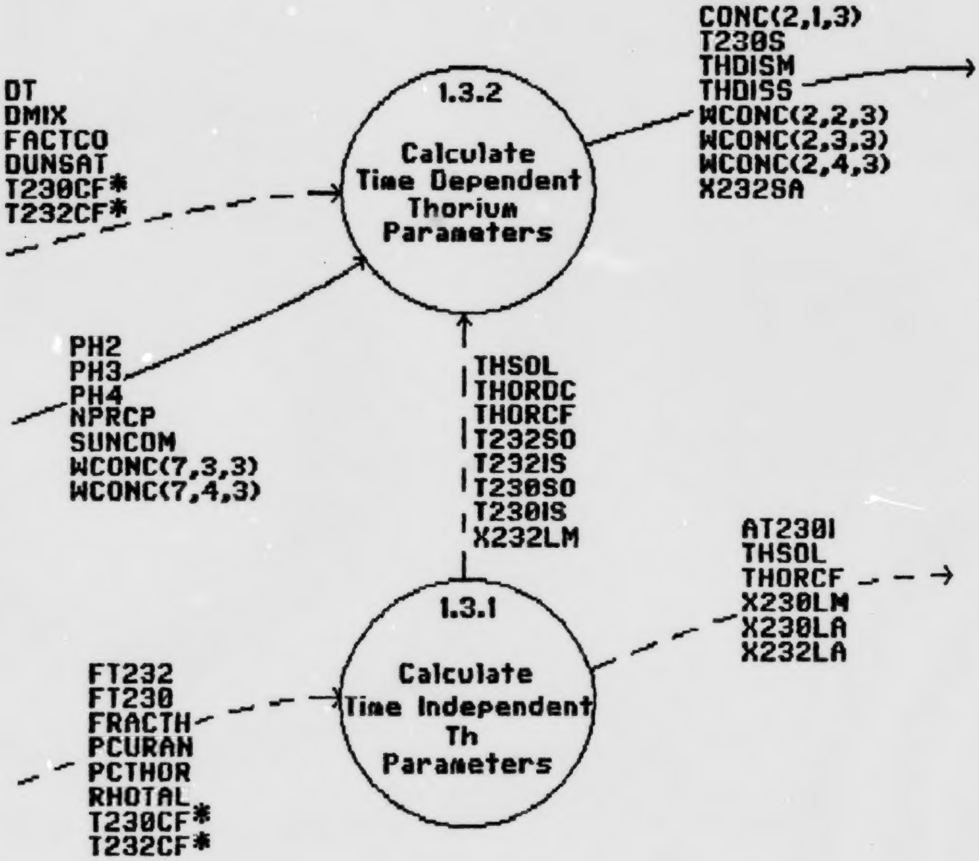
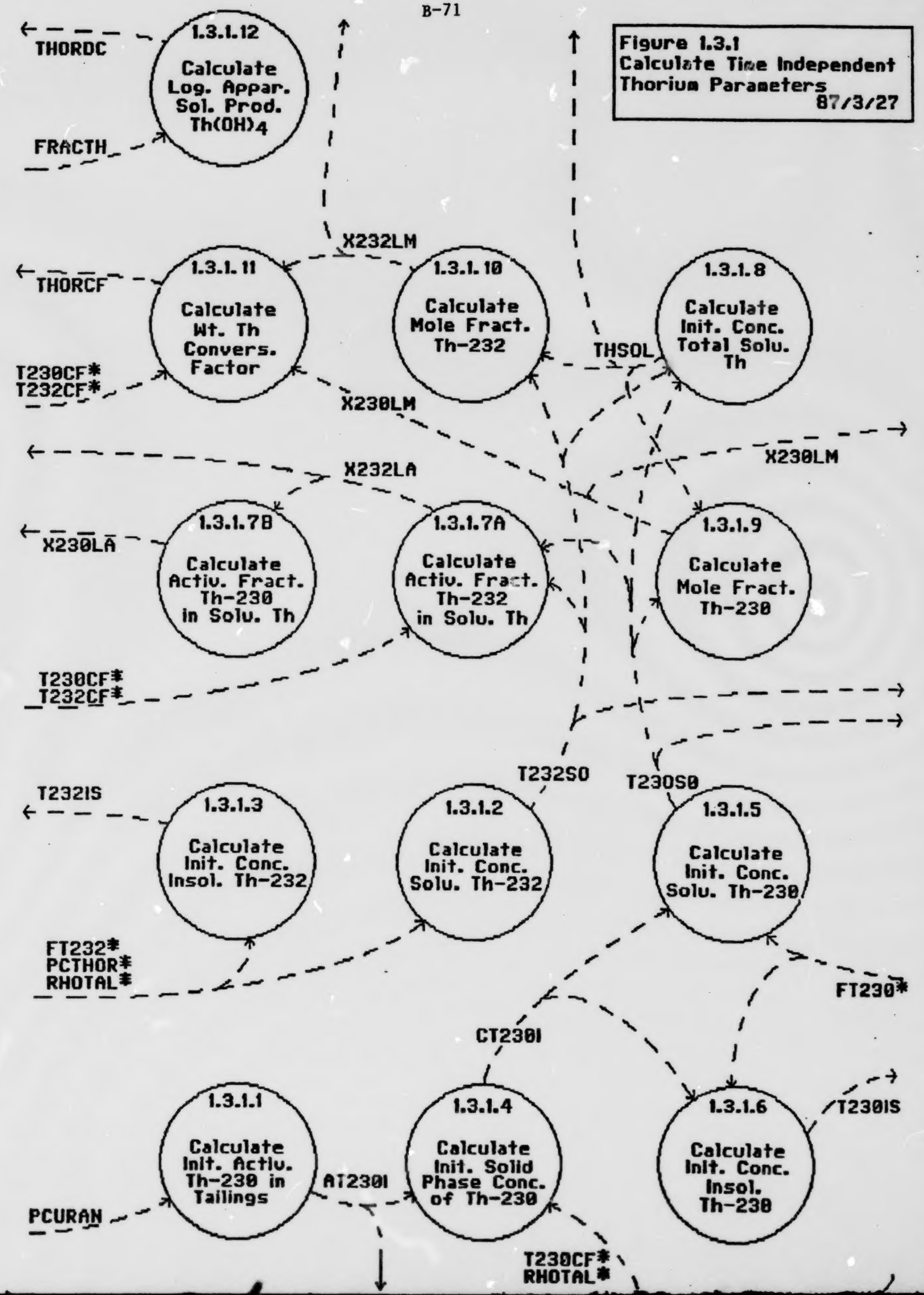

CONC(2,1,3)
T230S
THDISM
THDISS
WCONC(2,2,3)
WCONC(2,3,3)
WCONC(2,4,3)
X232SA
DT
DMIX
FACTCO
DUNSAT
T230CF*
T232CF*
1.3.2
Calculate
Time Dependent
Thorium
Parameters
PH2
PH3
PH4
NPRCP
SUNCOM
WCONC(7,3,3)
WCONC(7,4,3)
THSOL
THORDC
THORCF
T232SO
T232IS
T230SO
T230IS
X232LM
AT230I
THSOL
THORCF
X230LM
X230LA
X232LA
1.3.1
Calculate
Time Independent
Th
Parameters
FT232
FT230
FRACTH
PCURAN
PCTHOR
RHOTAL
T230CF*
T232CF*

Figure 1.3.1
Calculate Time Independent
Thorium Parameters
87/3/27


THORDC
1.3.1.12
Calculate Log. Appar. Sol. Prod. Th(OH)4
FRACTH
X232LM
THORCF
1.3.1.11
Calculate Wt. Th Convers. Factor
T230CF*
T232CF*
1.3.1.10
Calculate Mole Fract. Th-232
THSOL
1.3.1.8
Calculate Init. Conc. Total Solu. Th
X230LM
X230LM
X232LA
X230LA
1.3.1.7B
Calculate Activ. Fract. Th-230 in Solu. Th
1.3.1.7A
Calculate Activ. Fract. Th-232 in Solu. Th
1.3.1.9
Calculate Mole Fract. Th-230
T230CF*
T232CF*
T232SO
T230SO
T232IS
1.3.1.3
Calculate Init. Conc. Insol. Th-232
1.3.1.2
Calculate Init. Conc. Solu. Th-232
1.3.1.5
Calculate Init. Conc. Solu. Th-230
FT232*
PCTHOR*
RHOTAL*
FT230*
CT230I
1.3.1.1
Calculate Init. Activ. Th-230 in Tailings
AT230I
1.3.1.4
Calculate Init. Solid Phase Conc. of Th-230
1.3.1.6
Calculate Init. Conc. Insol. Th-230
T230IS
PCURAN
T230CF*
RHOTAL*

AT230I - INIT. ACTIV. TH-230 IN TAILINGS [Bq g^{-1}]. The initial activity of (solid) Th-230 in the tailings.

Figure 1.3.1.1
Calculate INIT. ACTIV.
TH-230 IN TAILINGS
(AT230I)

AU2380 - - -> AT230I

PCURAN - - -> AU2380

Short Name	Long Name	SI Unit	Source
AT230I	INIT. ACTIV. TH-230 IN TAILINGS	[Bq g^{-1}]	1.3.1.1
AU2380	INITIAL ACTIVITY U-238 IN ORE	[Bq g^{-1}]	(1.3.1.1)
PCURAN	MASS % U (AS U_3O_8) IN ORE	[-]	Sampled

$$\text{AT230I} = \text{AU2380} \qquad \text{(eqn. 3.7.13)}$$

$$\text{AU2380} = \left(\frac{\text{PCURAN}}{100}\right) * \left(\frac{714}{842}\right) * 1.22 \times 10^4 \qquad \text{(eqn. 3.7.2)}$$

Unit check:

AT230I [Bq g^{-1}] = [Bq g^{-1}]

AU2380 [-] * [g g^{-1}] * [Bq g^{-1}] = [Bq g^{-1}]

Note: "714" and "842" both have units of [g] (eqn. 3.7.2). "1.22×10^4" [Bq g^{-1}] is the activity of U-238 in natural uranium.

T232SO - INIT. CONC. SOLU. TH-232 [mol m^{-3}].
T232IS - INIT. CONC. INSOL. TH-232 [mol m^{-3}].
Initial concentration of soluble/insoluble Th-232 in the tailings.

Figures 1.3.1.2 and 1.3.1.3
Calculate INIT. CONC. SOLU. TH-232 AND INIT. CONC. INSOL. TH-232
(T232SO) and (T232IS)

CT232I FT232	- - ->	T232SO
CT232I FT232	- - ->	T232IS
RHOTAL PCTHOR	- - ->	CT232I

Short Name	Long Name	SI Unit	Source
CT232I	INIT. SOLID PHASE CONC. OF TH-232	[mol m^{-3}]	(1.3.1.2)
FT232	FRACT. TH-232 SOLUBLE	[-]	Sampled
PCTHOR	MASS % TH	[-]	Sampled
RHOTAL	TAILINGS BULK DENSITY	[g m^{-3}]	Sampled
T232IS	INIT. CONC. INSOL. TH-232	[mol m^{-3}]	1.3.1.3
T232SO	INIT. CONC. SOLU. TH-232	[mol m^{-3}]	1.3.1.2

$$\text{T232SO} = \text{FT232} * \text{CT232I} \qquad \text{(eqn. 3.7.20)}$$

$$\text{T232IS} = (1-\text{FT232}) * \text{CT232I} \qquad \text{(eqn. 3.7.22)}$$

$$\text{CT232I} = \left(\frac{\text{PCTHOR}}{100}\right) * \left(\frac{\text{RHOTAL}}{264}\right) \qquad \text{(eqn. 3.7.15)}$$

Unit check:

T232SO $[-] * [\text{mol m}^{-3}] = [\text{mol m}^{-3}]$

T232IS $[-] * [\text{mol m}^{-3}] = [\text{mol m}^{-3}]$

CT232I $[-] * [\text{g m}^{-3}] / [\text{g mol}^{-1}] = [\text{mol m}^{-3}]$

Note 1: In equation (3.7.15) the factor of 100 converts the percentage to a fraction, and the factor 264 is the molecular weight of ThO_2 [g mol^{-1}].

Note 2: The symbols $[\text{Th-232}_s]_{sol}$ and $[\text{Th-232}_s]_{insol}$, page 3-58, were assumed to be identical to $[\text{Th-232}_s]^{o}_{sol}$ and $[\text{Th-232}_s]^{o}_{insol}$, respectively (page 3-58 and Table A.3).

Figure 1.3.1.4
Calculate INIT. SOLID
PHASE CONC. OF TH-230
(CT230I)

CT230I - INIT. SOLID PHASE CONC. OF TH-230 [mol m-3]. Initial solid phase concentration of Th-230 in the tailings.

AT230I
RHOTAL - - -> CT230I
T230CF

Short Name	Long Name	SI Unit	Source
AT230I	INIT. ACTIV. TH-230 IN TAILINGS	$[\mathrm{Bq\ g^{-1}}]$	1.3.1.1
CT230I	INIT. SOLID PHASE CONC. OF TH-230	$[\mathrm{mol\ m^{-3}}]$	1.3.1.4
RHOTAL	TAILINGS BULK DENSITY	$[\mathrm{g\ m^{-3}}]$	Sampled
T230CF	TH-230 CONVERSION FACTOR	$[\mathrm{Bq\ mol^{-1}}]$	Sampled

$$\mathrm{CT230I} = \mathrm{AT230I} * \mathrm{RHOTAL} / \mathrm{T230CF} \qquad \text{(eqn. 3.7.14)}$$

Unit check:

$$\frac{[\mathrm{Bq\ g^{-1}}] * [\mathrm{g\ m^{-3}}]}{[\mathrm{Bq\ mol^{-1}}]} = [\mathrm{mol\ m^{-3}}]$$

T230SO - INIT. CONC. SOLU. TH-230 [mol m^{-3}].
T230IS - INIT. CONC. INSOL. TH-230 [mol m^{-3}].
Initial concentration of soluble/ insoluble Th-230 in the tailings.

Figures 1.3.1.5 and 1.3.1.6 Calculate INIT. CONC. SOLU. TH-230 and INIT. CONC. INSOL. TH-230 (T230SO) and (T230IS)

CT230I
FT230 - - -> T230SO

CT230I
FT230 - - -> T230IS

Short Name	Long Name	SI Unit	Source
CT230I	INIT. SOLID PHASE CONC. OF TH-230	[mol m^{-3}]	1.3.1.4
FT230	FRACT. TH-230 SOLUBLE	[-]	Sampled
T230IS	INIT. CONC. INSOL. TH-230	[mol m^{-3}]	1.3.1.6
T230SO	INIT. CONC. SOLU. TH-230	[mol m^{-3}]	1.3.1.5

$$T230SO = FT230 * CT230I \qquad \text{(eqn. 3.7.19)}$$

$$T230IS = (1-FT230) * CT230I \qquad \text{(eqn. 3.7.21)}$$

Unit check:

T230SO $[-] * [\text{mol m}^{-3}] = [\text{mol m}^{-3}]$

T230IS $[-] * [\text{mol m}^{-3}] = [\text{mol m}^{-3}]$

Note: The symbols $[\text{Th-230}_s]_{sol}$, $[\text{Th-230}_s]_{insol}$ (page 3-58) were assumed to be identical to $[\text{Th-230}_s]^{\circ}_{sol}$ and $[\text{Th-230}_s]^{\circ}_{insol}$, respectively (page 3-58 and Table A.3).

X232LA - ACTIV. FRACT. TH-232 IN SOLU. TH [-].
The fraction of Th-232 in soluble thorium on the basis of activity.

X230LA - ACTIV. FRACT. TH-230 IN SOLU. TH [-].
The fraction of Th-230 in soluble thorium on the basis of activity.

Figure 1.3.1.7A
Calculate ACTIV. FRACT. TH-232 IN SOLU. TH (X232LA)

Figure 1.3.1.7B
Calculate ACTIV. FRACT. TH-230 IN SOLU. TH (X230LA)

T230CF
T230SO
T232SO - - -> X232LA
T232CF

X232LA - - -> X230LA

Short Name	Long Name	SI Unit	Source
T230CF	TH-230 CONVERSION FACTOR	$[\mathrm{Bq\ mol^{-1}}]$	Sampled
T230SO	INIT. CONC. SOLU. TH-230	$[\mathrm{mol\ m^{-3}}]$	1.3.1.5
T232CF	TH-232 CONVERSION FACTOR	$[\mathrm{Bq\ mol^{-1}}]$	Sampled
T232SO	INIT. CONC. SOLU. TH-232	$[\mathrm{mol\ m^{-3}}]$	1.3.1.2
X230LA	ACTIV. FRACT. TH-230 IN SOLU. TH	[-]	1.3.1.7B
X232LA	ACTIV. FRACT. TH-232 IN SOLU. TH	[-]	1.3.1.7A

$$\mathrm{X232LA} = \frac{\mathrm{T232SO} * \mathrm{T232CF}}{\mathrm{T230SO} * \mathrm{T230CF} + \mathrm{T232SO} * \mathrm{T232CF}}$$

(eqns. 3.7.26 and 3.7.29; see Note 2)

$$\mathrm{X230LA} = 1\text{-}\mathrm{X232LA}$$

(Note 3)

Unit check:

$$\frac{[\mathrm{mol\ m^{-3}}] * [\mathrm{Bq\ mol^{-1}}]}{[\mathrm{mol\ m^{-3}}] * [\mathrm{Bq\ mol^{-1}}] + [\mathrm{mol\ m^{-3}}] * [\mathrm{Bq\ mol^{-1}}]} = [-]$$

Note 1: It is assumed $[\mathrm{Th\text{-}230}]^{\circ}_{sol}$ is identical to $[\mathrm{Th\text{-}230_s}]^{\circ}_{sol} \equiv$ T230SO, and $[\mathrm{Th\text{-}232}]^{\circ}_{sol}$ is identical to $[\mathrm{Th\text{-}232_s}]^{\circ}_{sol} \equiv$ T232SO.

Note 2: Calculated from

$XA_{Th\text{-}232/Th,sol} = [\mathrm{Th\text{-}232_s}]^{\circ}_{sol}$ $\mathrm{T232CF}/a^{\circ}_{Th,sol}$ (equation (3.7.29) using $a^{\circ}_{Th,sol}$ as defined by equation (3.7.26).

Note 3: By definition X230LA + X232LA = 1.

THSOL - INIT. CONC. TOTAL SOLU. TH [mol m^{-3}].
The initial concentration of total soluble thorium (Th-230 + Th-232) in the tailings.

Figure 1.3.1.8
Calculate INIT. CONC. TOTAL SOLU. TH (THSOL)

$$\begin{tikzcd} \begin{matrix} \text{T230SO} \\ \text{T232SO} \end{matrix} \arrow[r, dashed] & \text{THSOL} \end{tikzcd}$$

Short Name	Long Name	SI Unit	Source
T230SO	INIT. CONC. SOLU. TH-230	[mol m^{-3}]	1.3.1.5
T232SO	INIT. CONC. SOLU. TH-232	[mol m^{-3}]	1.3.1.2
THSOL	INIT. CONC. TOTAL SOLU. TH	[mol m^{-3}]	1.3.1.8

$$\text{THSOL} = \text{T230SO} + \text{T232SO} \qquad \text{(eqn. 3.7.23)}$$

Unit check:

THSOL [mol m^{-3}] + [mol m^{-3}] = [mol m^{-3}]

X230LM - MOLE FRACT. TH-230 [-]. Mole fraction of Th-230 in soluble thorium.
X232LM - MOLE FRACT. TH-232 [-]. Mole fraction of Th-232 in soluble thorium.

Figures 1.3.1.9 and 1.3.1.10 Calculate MOLE FRACT. TH-230 (X230LM) and MOLE FRACT. TH-232 (X232LM)

T230SO
THSOL - - -> X230LM

THSOL
T232SO - - -> X232LM

Short Name	Long Name	SI Unit	Source
T230SO	INIT. CONC. SOLU. TH-230	[mol m^{-3}]	1.3.1.5
T232SO	INIT. CONC. SOLU. TH-232	[mol m^{-3}]	1.3.1.2
THSOL	INIT. CONC. TOTAL SOLU. TH	[mol m^{-3}]	1.3.1.8
X230LM	MOLE FRACT. TH-230	[-]	1.3.1.9
X232LM	MOLE FRACT. TH-232	[-]	1.3.1.10

$$X230LM = T230SO/THSOL \qquad \text{(eqn. 3.7.27)}$$

$$X232LM = T232SO/THSOL \qquad \text{(eqn. 3.7.28)}$$

Unit check:

X230LM [mol m^{-3}] / [mol m^{-3}] = [-]

X232LM [mol m^{-3}] / [mol m^{-3}] = [-]

Note: By definition X230LM + X232LM = 1.

Figure 1.3.1.11
Calculate WT. TH
CONVERS. FACTOR
(THORCF)

THORCF - WT. TH CONVERS. FACTOR [Bq mol^{-1}]. The weighted liquid phase thorium conversion factor for solutions containing both Th-230 and Th-232.

T230CF
X230LM
X232LM - - -> THORCF
T232CF

Short Name	Long Name	SI Unit	Source
T230CF	TH-230 CONVERSION FACTOR	[Bq mol^{-1}]	Sampled
T232CF	TH-232 CONVERSION FACTOR	[Bq mol^{-1}]	Sampled
THORCF	WT. TH CONVERS. FACTOR	[Bq mol^{-1}]	1.3.1.11
X230LM	MOLE FRACT. TH-230	[-]	1.3.1.9
X232LM	MOLE FRACT. TH-232	[-]	1.3.1.10

$$\mathrm{THORCF} = \mathrm{X230LM} * \mathrm{T230CF} + \mathrm{X232LM} * \mathrm{T232CF} \qquad \text{(eqn. 3.7.31)}$$

Unit check:

$$[-] * [\mathrm{Bq\ mol^{-1}}] + [-] * [\mathrm{Bq\ mol^{-1}}] = [\mathrm{Bq\ mol^{-1}}]$$

Note: Equation (3.7.31) was modified using the definition X230LM + X232LM = 1.

THORDC - LOG APPAR. SOL. PROD. $TH(OH)_4$ [-].
The averaged (apparent) value of the logarithm (base 10) of the solubility product of a mixture of amorphous and crystalline thorium hydroxide.

Figure 1.3.1.12
Calculate LOG APPAR. SOL. PROD. $TH(OH)_4$ (THORDC)

FRACTH - - -> THORDC

Short Name	Long Name	SI Unit	Source
FRACTH	FRAC. OF $TH(OH)_4$ CRYSTALLINE	[-]	Sampled
THORDC	LOG APPAR. SOL. PROD. $TH(OH)_4$	[-]	1.3.1.12

$$THORDC = 1.78 * FRACTH + 6.3 * (1 - FRACTH) \qquad \text{(eqn. 3.9.3)}$$

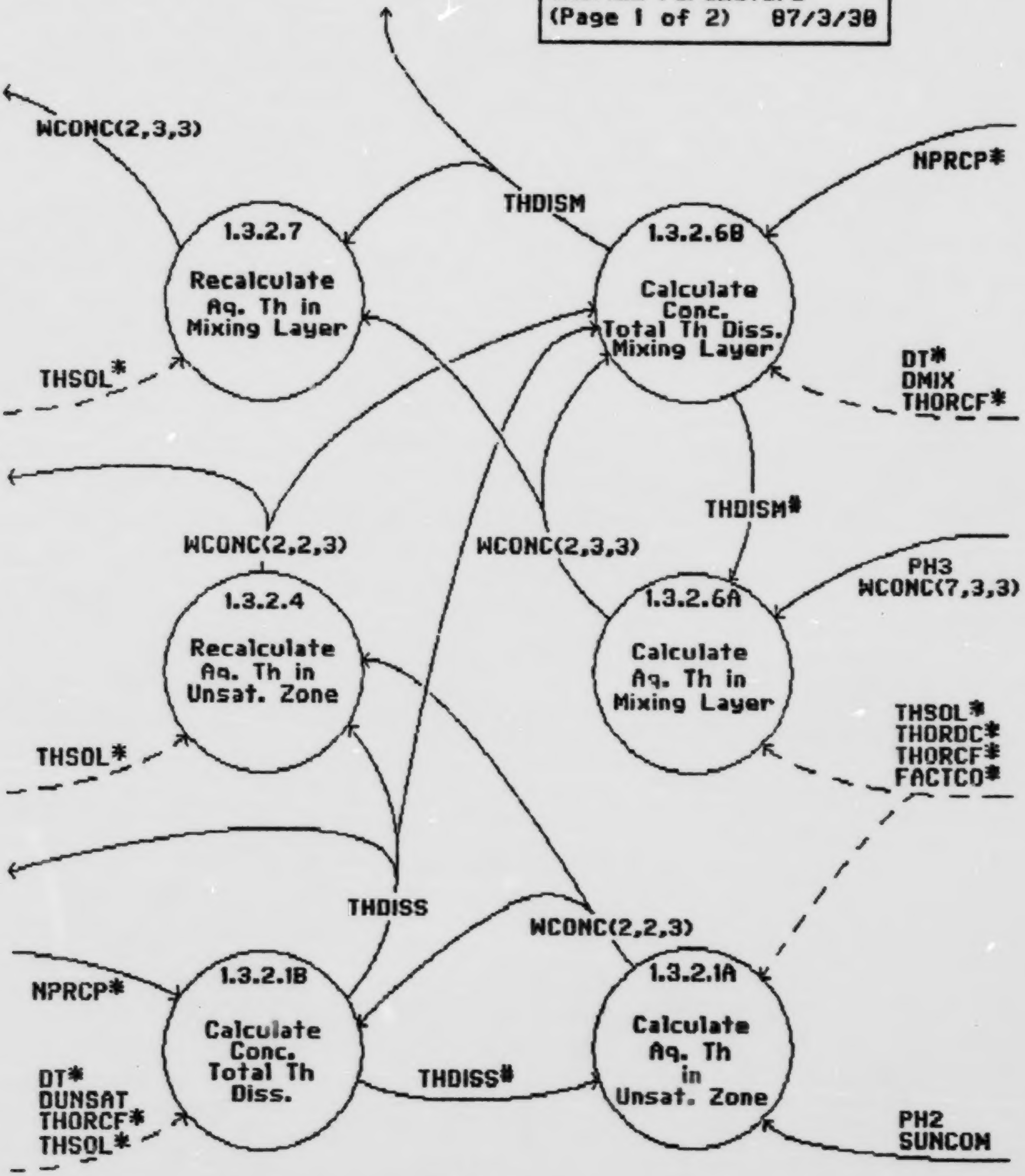
Unit check: All dimensionless by definition.

Note 1: The definition of $X_{Th,c}$ given on page 3.72 is misleading. It is the logarithms (base 10) of the constants that are being averaged.

Note 2: Where THORDC is used (e.g., eqn 3.9.1), the value of $10^{K_{Th}}$ has units of $mol^{-3}dm^{9}$.

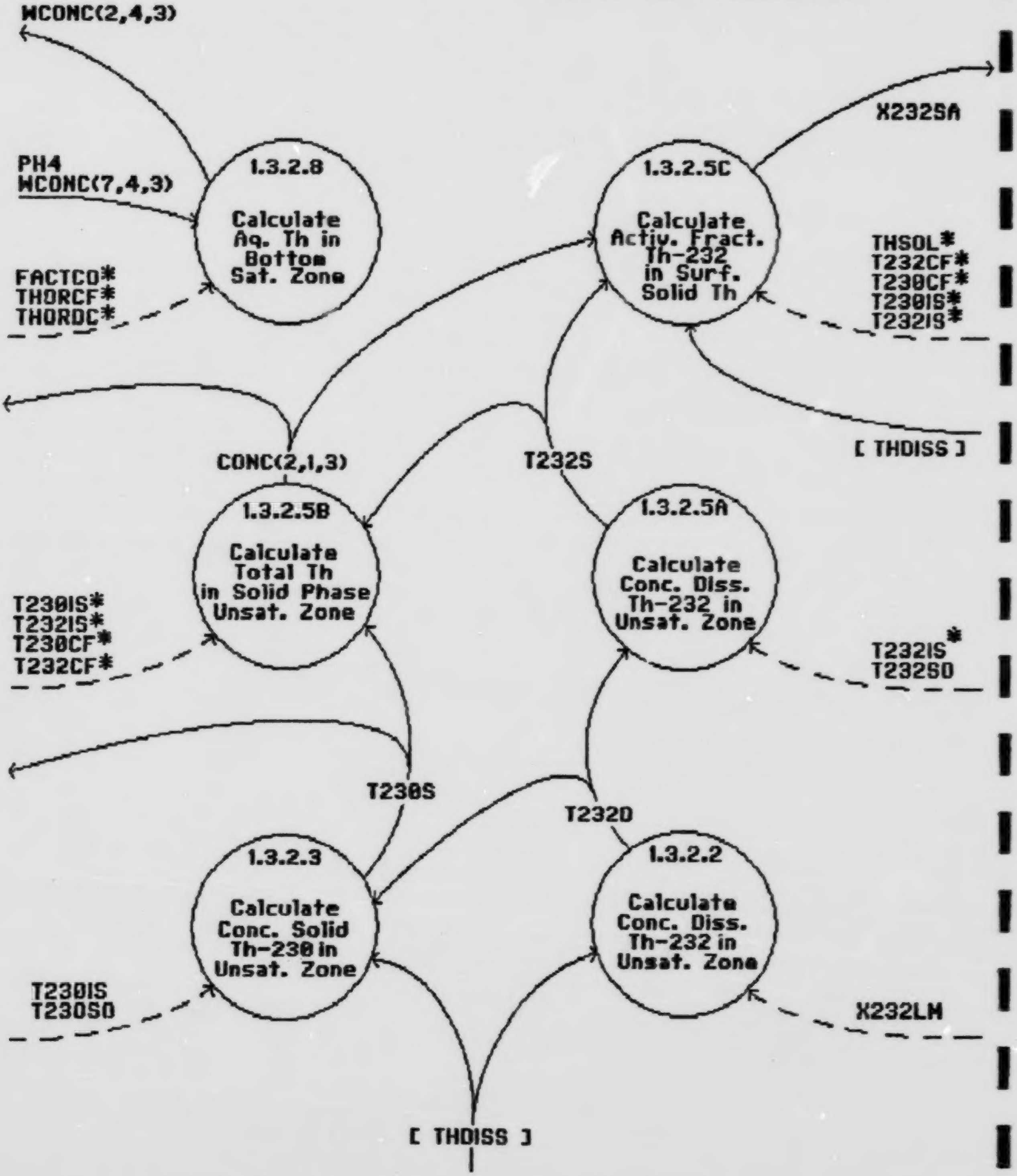
Note 3: K_{TH} is assumed identical to K_{Th}.

Figure 1.3.2
Calculate Time Dependent
Thorium Parameters
(Page 1 of 2) 87/3/30


WCONC(2,3,3)
THDISM
NPRCP*
1.3.2.7
Recalculate
Aq. Th in
Mixing Layer
1.3.2.6B
Calculate
Conc.
Total Th Diss.
Mixing Layer
THSOL*
DT*
DMIX
THORCF*
THDISM#
WCONC(2,2,3)
WCONC(2,3,3)
PH3
WCONC(7,3,3)
1.3.2.4
Recalculate
Aq. Th in
Unsat. Zone
1.3.2.6A
Calculate
Aq. Th in
Mixing Layer
THSOL*
THSOL*
THORDC*
THORCF*
FACTCO*
THDISS
WCONC(2,2,3)
NPRCP*
1.3.2.1B
Calculate
Conc.
Total Th
Diss.
1.3.2.1A
Calculate
Aq. Th
in
Unsat. Zone
THDISS#
DT*
DUNSAT
THORCF*
THSOL*
PH2
SUNCON

Note: THDISM# and THDISS# refer to values of the variables at the previous time step.

Figure 1.3.2
Calculate Time Dependent
Thorium Parameters
(Page 2 of 2) 87/3/30


WCONC(2,4,3)
PH4
WCONC(7,4,3)
1.3.2.8
Calculate Aq. Th in Bottom Sat. Zone
FACTCO*
THORCF*
THORDC*
X232SA
1.3.2.5C
Calculate Activ. Fract. Th-232 in Surf. Solid Th
THSOL*
T232CF*
T230CF*
T230IS*
T232IS*
[THDISS]
CONC(2,1,3)
T232S
1.3.2.5B
Calculate Total Th in Solid Phase Unsat. Zone
T230IS*
T232IS*
T230CF*
T232CF*
1.3.2.5A
Calculate Conc. Diss. Th-232 in Unsat. Zone
T232IS*
T232SD
T230S
T232D
1.3.2.3
Calculate Conc. Solid Th-230 in Unsat. Zone
T230IS
T230SD
1.3.2.2
Calculate Conc. Diss. Th-232 in Unsat. Zone
X232LM
[THDISS]

Note: THDISS is from Part 1 of this figure.

Figure 1.3.2.1A
Calculate AQ. TH IN UNSAT. ZONE (WCONC(2,2,3))

WCONC(2,2,3) - AQ. TH IN UNSAT. ZONE [Bq m^{-3}]. The concentration of thorium in the aqueous phase at the bottom of the unsaturated zone.

THORCF
THORDC
THSOL
FACTCO
- - -> WCONC(2,2,3) <——
SUNCOM
THDISS(t-Δt)
PH2

Short Name	Long Name	SI Unit	Source
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
PH2	PH LAYER 2	[-]	1.1.2.8
SUNCOM	CONC. UNCOMP. SO_4 BOTTOM UNSAT. ZONE	[mol dm^{-3}]	1.1.2.12
THDISS	CONC. TOTAL TH DISS.	[mol m^{-3}]	1.3.2.1B
THORCF	WT. TH CONVERS. FACTOR	[Bq mol^{-1}]	1.3.1.11
THORDC	LOG APPAR. SOL. PROD. $TH(OH)_4$	[-]	1.3.1.12
THSOL	INIT. CONC. TOTAL SOLU. TH	[mol m^{-3}]	1.3.1.8
WCONC(2,2,3)	AQ. TH IN UNSAT. ZONE	[Bq m^{-3}]	1.3.2.1A, 1.3.2.4

(a) If THDISS(t-Δt) < THSOL

$$\begin{aligned} \text{WCONC}(2,2,3) = {} & \frac{10^3 * \text{THORCF} * 10^{(\text{THORDC}-4*\text{PH2})}}{(\text{FACTCO})^4} * \Big\{1 + (\text{FACTCO})^{1.75} \\ & * 10^{(\text{PH2}-3.2)} + (\text{FACTCO})^3 * 10^{(2*\text{PH2}-6.93)} + (\text{FACTCO})^{3.75} \\ & * 10^{(3*\text{PH2}-11.7)} + (\text{FACTCO})^4 * \Big[10^{(4*\text{PH2}-15.9)} + 10^{5.45} * \text{SUNCOM}\Big] \\ & + (\text{FACTCO})^6 * 10^{9.73} * (\text{SUNCOM})^2\Big\} \end{aligned}$$

(eqn. 3.9.1; (see Notes 1 & 2)

(b) Then, if $\text{WCONC}(2,2,3) > 10^3 * \text{THORCF} * 5 * 10^{-5}$

$$\text{WCONC}(2,2,3) = 10^3 * \text{THORCF} * 5 * 10^{-5}$$ (eqn. 3.9.2, see Note 3)

(c) If THDISS(t-Δt) $\geq$ THSOL

$$\text{WCONC}(2,2,3) = 0$$ (eqn. 3.9.12)

Unit check:

Units of terms in "[ ]" are assumed to be in dimensionless

$$\text{WCONC}(2,2,3){:}\quad \frac{[\text{dm}^3\ \text{m}^{-3}] * [\text{Bq mol}^{-1}] * [\text{mol dm}^{-3}] * [-]}{[-]} = [\text{Bq m}^{-3}]$$

Note 1: The factors 10^3 [dm m^{-3}] and THORCF [Bq mol^{-1}] are necessary to obtain WCONC(2,2,3) in [Bq m^{-3}].

Note 2: SENES text indicates pH2 ≡ pH in equation (3.9.1).

Note 3: Equation (3.9.2) has been modified by the factor (10^3 * THORCF) so the comparison term has units of [Bq m^{-3}], as has WCONC(2,2,3) (see also Note 1).

Figure 1.3.2.1B
Calculate
CONC. TOTAL TH DISS.
(THDISS)

THDISS - CONC. TOTAL TH DISS. [mol m^{-3}]. The concentration of total thorium (Th-230 and Th-232) that has dissolved in the unsaturated zone to TIME=t.

THORCF
THSOL
DUNSAT
DT≡Δt
- - -> THDISS(t) <—— THDISS(t-Δt)
NPRCP
WCONC(2,2,3)

Short Name	Long Name	SI Unit	Source
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled
THDISS	CONC. TOTAL TH DISS.	[mol m^{-3}]	1.3.2.1B
THORCF	WT. TH CONVERS. FACTOR	[Bq mol^{-1}]	1.3.1.11
THSOL	INIT. CONC. TOTAL SOLU. TH	[mol m^{-3}]	1.3.1.8
WCONC(2,2,3)	AQ. TH IN UNSAT. ZONE	[Bq m^{-3}]	1.3.2.1A

(a) If THDISS < THSOL at Time=(t-Δt)

from the finite difference equation

$$\mathrm{THDISS}(t) = \mathrm{THDISS}(t-\Delta t) + \frac{\mathrm{NPRCP} * \mathrm{DT} * \mathrm{WCONC}(2,2,3)}{\mathrm{DUNSAT} * \mathrm{THORCF}}$$

(eqn. 3.9.4)

(b) If THDISS $\geq$ THSOL at Time=t

THDISS = THSOL (discussion near eqn. 3.9.12)

Unit check:

(a) $$\frac{[\mathrm{m\ a^{-1}}] * [\mathrm{a}] * [\mathrm{Bq\ m^{-3}}]}{[\mathrm{m}] * [\mathrm{Bq\ mol^{-1}}]} = [\mathrm{mol\ m^{-3}}]$$

(b) $[\mathrm{mol\ m^{-3}}] = [\mathrm{mol\ m^{-3}}]$

Note 1: Factor of THORCF is required because WCONC(2,2,3) has units [Bq m^{-3}].

Note 2: Unit check requires WCONC(2,2,3) in [Bq m^{-3}], Table A.3 gives [Bq m^{-3}], pg. 3-73 gives [mol m^{-3}], equation (3.9.1) gives WCONC(2,2,3) in [mol dm^{-3}]. See discussion SENES pg 3-72 - 3-74 and elsewhere. We have kept THDISS in [mol m^{-3}].

Note 3: $[\mathrm{Th}_L]_{\lambda w}$ is assumed to be in the numerator of equation 3.9.4 in order to maintain the unit check.

Note 4: THDISS = 0.0 at TIME=-Δt (SENES letter 1987-01-27).

Note 5: Inspection of the UTAP2 code shows that THDISS=0 at t=0. Apparently this condition holds for t<0 as well. (BWG, 87-04-02)

Figure 1.3.2.2
Calculate CONC. DISS.
TH-232 IN UNSAT. ZONE
(T232D)

T232D - CONC. DISS. TH-232 IN UNSAT. ZONE [mol m^{-3}]. The total concentration of Th-232 dissolved in the unsaturated zone to TIME=t.

X232LM - - -> T232D <—— THDISS

Short Name	Long Name	SI Unit	Source
T232D	CONC. DISS. TH-232 IN UNSAT. ZONE	[mol m^{-3}]	1.3.2.2
THDISS	CONC. TOTAL TH DISS.	[mol m^{-3}]	1.3.2.1
X232LM	MOLE FRACT. TH-232	[-]	1.3.1.10

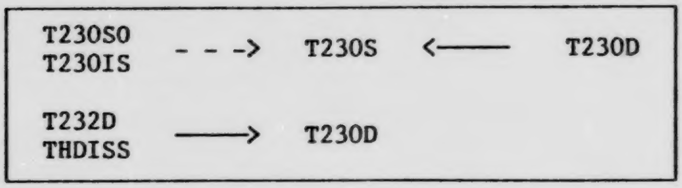
$$T232D = THDISS * X232LM \qquad \text{(eqn. 3.9.5)}$$

Unit check:

$$[mol\ m^{-3}] * [-] = [mol\ m^{-3}]$$

T230S - CONC. SOLID TH-230 IN UNSAT. ZONE [mol m^{-3}]. The solid phase concentration of Th-230 in the unsaturated zone.

Figure 1.3.2.3
Calculate CONC. SOLID
TH-230 IN UNSAT. ZONE
(T230S)



Short Name	Long Name	SI Unit	Source
T230D	CONC. DISS. TH-230 IN UNSAT. ZONE	[mol m^{-3}]	(1.3.2.3)
T230IS	INIT. CONC. INSOL. TH-230	[mol m^{-3}]	1.3.1.6
T230S	CONC. SOLID TH-230 IN UNSAT. ZONE	[mol m^{-3}]	1.3.2.3
T230SO	INIT. CONC. SOLU. TH-230	[mol m^{-3}]	1.3.1.5
T232D	CONC. DISS. TH-232 IN UNSAT. ZONE	[mol m^{-3}]	1.3.2.2
THDISS	CONC. TOTAL TH DISS.	[mol m^{-3}]	1.3.2.1

$$\text{T230D} = \text{THDISS} - \text{T232D} \qquad \text{(eqn. 3.9.6)}$$

$$\text{T230S} = \text{T230IS} + \text{T230SO} - \text{T230D} \qquad \text{(eqn. 3.9.7)}$$

Unit check:

T230D: $[\text{mol m}^{-3}] - [\text{mol m}^{-3}] = [\text{mol m}^{-3}]$

T230S: $[\text{mol m}^{-3}] + [\text{mol m}^{-3}] - [\text{mol m}^{-3}] = [\text{mol m}^{-3}]$

Note: Assumed $[\text{Th-230}]^{\circ}_{sol} \equiv [\text{Th-230}_s]^{\circ}_{sol}$
and $[\text{Th-230}]^{\circ}_{insol} \equiv [\text{Th-230}_s]^{\circ}_{insol}$

WCONC(2,2,3) - AQ. TH IN UNSAT. ZONE [Bq m^{-3}]. The concentration of thorium in the aqueous phase at the bottom of the unsaturated zone.

Figure 1.3.2.4
Recalculate AQ. TH
IN UNSAT. ZONE
(WCONC(2,2,3))

THSOL - - -> WCONC(2,2,3) <—— WCONC(2,2,3)
THDISS

Short Name	Long Name	SI Unit	Source
THDISS	CONC. TOTAL TH DISS.	[mol m^{-3}]	1.3.2.1B
THSOL	INIT. CONC. TOTAL SOLU.TH	[mol m^{-3}]	1.3.1.8
WCONC(2,2,3)	AQ. TH IN UNSAT. ZONE	[Bq m^{-3}]	1.3.2.1A & 1.3.2.4

(a) If THDISS $\geq$ THSOL

$$\text{WCONC}(2,2,3) = 0.0 \qquad \text{(eqn. 3.9.12)}$$

(b) If THDISS < THSOL

$$\text{WCONC}(2,2,3) = \text{WCONC}(2,2,3)$$

Unit check:

$$[\text{Bq m}^{-3}] = [\text{Bq m}^{-3}]$$

Figure 1.3.2.5A
Calculate CONC. SOLID
TH-232 IN UNSAT. ZONE
(T232S)

T232S - CONC. SOLID TH-232 IN UNSAT. ZONE [mol m^{-3}]. The solid phase concentration of Th-232 in the unsaturated zone.

T232IS
T232SO - - -> T232S <—— T232D

Short Name	Long Name	SI Unit	Source
T232D	CONC. DISS. TH-232 IN UNSAT. ZONE	[mol m^{-3}]	1.3.2.2
T232IS	INIT. CONC. INSOL. TH-232	[mol m^{-3}]	1.3.1.3
T232S	CONC. SOLID TH-232 IN UNSAT. ZONE	[mol m^{-3}]	1.3.2.5A
T232SO	INIT. CONC. SOLU. TH-232	[mol m^{-3}]	1.3.1.2

$$\text{T232S} = \text{T232IS} + \text{T232SO} - \text{T232D} \qquad \text{(eqn. 3.9.8)}$$

Unit check:

$$[\text{mol m}^{-3}] + [\text{mol m}^{-3}] - [\text{mol m}^{-3}] = [\text{mol m}^{-3}]$$

Note: It is assumed that:

$$[\text{Th-232}]^{\circ}_{insol} \equiv [\text{Th-232}_s]^{\circ}_{insol}$$

$$[\text{Th-232}]^{\circ}_{sol} \equiv [\text{Th-232}_s]^{\circ}_{sol}$$

CONC(2,1,3) - TOTAL TH IN SOLID PHASE, UNSAT. ZONE [Bq m^{-3}]. Concentration of total thorium in the solid phase of the unsaturated zone.

Figure 1.3.2.5B
Calculate TOTAL TH IN SOLID PHASE, UNSAT. ZONE (CONC(2,1,3))

```
T230CF
T232CF                                 T230S
T230IS   - - ->  CONC(2,1,3)  <------  T232S
T232IS
```

Short Name	Long Name	SI Unit	Source
CONC(2,1,3)	TOTAL TH IN SOLID PHASE, UNSAT. ZONE	[Bq m^{-3}]	1.3.2.5B
T230CF	TH-230 CONVERSION FACTOR	[Bq mol^{-1}]	Sampled
T230IS	INIT. CONC. INSOL. TH-230	[mol m^{-3}]	1.3.1.6
T230S	CONC. SOLID TH-230 IN UNSAT. ZONE	[mol m^{-3}]	1.3.2.3
T232CF	TH-232 CONVERSION FACTOR	[Bq mol^{-1}]	Sampled
T232IS	INIT. CONC. INSOL. TH-232	[mol m^{-3}]	1.3.1.3
T232S	CONC. SOLID TH-232 IN UNSAT. ZONE	[mol m^{-3}]	1.3.2.5A

CONC(2,1,3) = T230S * T230CF + T232S * T232CF (eqn. 3.9.10; see Notes)

Unit check:
[mol m^{-3}] * [Bq mol^{-1}] + [mol m^{-3}] * [Bq mol^{-1}] = [Bq m^{-3}]

Note 1: SENES Vol. 3 indicates equation (3.9.10) should be used if THDISS < THSOL and equation (3.9.13) if THDISS = THSOL.

Note 2: Inspection of the UTAP2 code shows that CONC(2,1,3) is calculated as follows:
(a) If THDISS=THSOL at any time,
CONC(2,1,3) = T232IS * T232CF + T230IS * T230CF
(b) If THDISS<THSOL, use eqn. (3.9.10) as above.
Note that eqn. (3.9.10) does not simplify to eqn. (3.9.13) when THDISS=THSOL, as expected. These changes are implemented in SYVAC3-UT2. (BWG, 87-05-04)

X232SA - ACTIV. FRACT. TH-232 IN SURF. SOLID TH [-]. The fraction of Th-232 in solid thorium in the unsaturated zone (on the basis of activity).

Figure 1.3.2.5C
Calculate ACTIV. FRACT.
TH-232 IN SURF. SOLID TH
(X232SA)

```
T230CF
T230IS                                CONC(2,1,3)
T232CF  - - ->  X232SA  <------   T232S
T232IS                                THDISS
THSOL
```

Short Name	Long Name	SI Unit	Source
CONC(2,1,3)	TOTAL TH IN SOLID PHASE, UNSAT. ZONE	$[Bq\ m^{-3}]$	1.3.2.5B
T230CF	TH-230 CONVERSION FACTOR	$[Bq\ mol^{-1}]$	Sampled
T230IS	INIT. CONC. INSOL. TH-230	$[mol\ m^{-3}]$	1.3.1.6
T232CF	TH-232 CONVERSION FACTOR	$[Bq\ mol^{-1}]$	Sampled
T232IS	INIT. CONC. INSOL. TH-232	$[mol\ m^{-3}]$	1.3.1.3
T232S	CONC. SOLID TH-232 IN UNSAT. ZONE	$[mol\ m^{-3}]$	1.3.2.5A
THDISS	CONC. TOTAL TH DISS.	$[mol\ m^{-3}]$	1.3.2.1B
THSOL	INIT. CONC. TOTAL SOLU. TH	$[mol\ m^{-3}]$	1.3.1.8
X232SA	ACTIV. FRACT. TH-232 IN SURF. SOLID TH	[-]	1.3.2.5C

X232SA = T232S * T232CF / CONC(2,1,3) (eqn. 3.9.11; see Note 2)

Unit check:

$$\frac{[mol\ m^{-3}] * [Bq\ mol^{-1}]}{[Bq\ m^{-3}]} = [-]$$

Note 1: As described in SENES Vol. 3, pg 3-74, a simpler equation (3.9.14) can be used if THDISS = THSOL. However equation (3.9.11) is also valid for that condition.

Note 2: Inspection of the UTAP2 code shows that X232SA is given, at $t \leq 0$, by the initial condition:
X232SA = T232IS * T232CF / (T232IS * T232CF + T230IS * T230CF)
This modified equation has been installed in SYVAC3-UT2. (BWG, 87-04-13)

Note 3: Inspection of the UTAP2 code shows that X232SA is given by the following logic:
(a) For t=0, use Note 2.
(b) For t>0 and THDISS<THSOL, use eqn. (3.9.11) as shown in this DDD.
(c) For t>0 and $THDISS \geq THSOL$, use the expression in Note 2. This condition also requires that THDISS and THSOL be passed to this DDD.
(BWG, 87-05-04)

WCONC(2,3,3) - AQ. TH IN MIXING LAYER [Bq m^{-3}]. The concentration of thorium in the aqueous phase in the mixing layer of the saturated zone.

Figure 1.3.2.6A
Calculate AQ. TH IN
MIXING LAYER
(WCONC(2,3,3))

```
THSOL                                        THDISM(t-Δt)
THORCF    - - ->   WCONC(2,3,3)   <-----     PH3
FACTCO                                       WCONC(7,3,3)
THORDC
```

Short Name	Long Name	SI Unit	Source
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
PH3	PH LAYER 3	[-]	1.1.4.8
THDISM	CONC. TOTAL TH DISS. MIXING LAYER	[mol m^{-3}]	1.3.2.6B
THORCF	WT. TH CONVERS. FACTOR	[Bq mol^{-1}]	1.3.1.11
THORDC	LOG APPAR. SOL. PROD. $TH(OH)_4$	[-]	1.3.1.12
THSOL	INIT. CONC. TOTAL SOLU. TH	[mol m^{-3}]	1.3.1.8
WCONC(2,3,3)	AQ. TH IN MIXING LAYER	[Bq m^{-3}]	1.3.2.6A
WCONC(7,3,3)	CONC. OF SO_4 AQ. IN MIXING LAYER	[mol m^{-3}]	1.1.4.6

(a) If THDISM(t-Δt) < THSOL

$$\mathrm{WCONC(2,3,3)} = \frac{1000.\ *\ \mathrm{THORCF}\ *\ 10^{(\mathrm{THORDC}-4*\mathrm{PH3})}}{(\mathrm{FACTCO})^{4.0}} * \Big\{1 + (\mathrm{FACTCO})^{1.75}$$

$$*10^{(\mathrm{PH3}-3.2)} + (\mathrm{FACTCO})^{3} * 10^{(2*\mathrm{PH3}-6.93)} + (\mathrm{FACTCO})^{3.75} * 10^{(3*\mathrm{PH3}-11.7)}$$

$$+ (\mathrm{FACTCO})^{4} * 10^{(4*\mathrm{PH3}-15.9)} + (\mathrm{FACTCO})^{4} * 10^{5.45} * \mathrm{WCONC(7,3,3)} / 10^{3}$$

$$+ (\mathrm{FACTCO})^{6} * 10^{9.73} * \mathrm{WCONC(7,3,3)} * \mathrm{WCONC(7,3,3)} / 10^{6}\Big\} \qquad \text{(eqn. 3.9.16)}$$

If $\mathrm{WCONC(2,3,3)} > 1000 * \mathrm{THORCF} * 5 * 10^{-5}$

$$\mathrm{WCONC(2,3,3)} = 1000 * \mathrm{THORCF} * 5 * 10^{-5} \qquad \text{(below eqn. 3.9.16)}$$

(b) If THDISM(t-Δt) ≥ THSOL

$$\mathrm{WCONC(2,3,3)} = 0 \qquad \text{(eqn. 3.9.19)}$$

Unit check:

(a) $[dm^3\ m^{-3}] * [Bq\ mol^{-1}] * [mol\ dm^{-3}] = [Bq\ m^{-3}]$

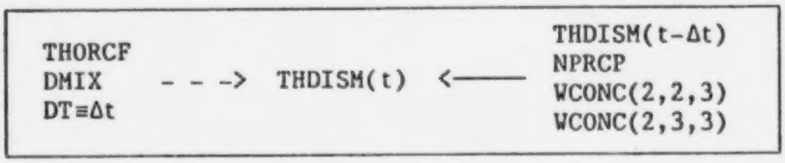
Note 1: The factors 10^3 [dm^3 m^{-3}] and THORCF [Bq mol^{-1}] are necessary to obtain WCONC(2,3,3) in [Bq m^{-3}].

Note 2: The factor in brackets { } is assumed to be dimensionless.

Note 3: Inspection of the UTAP2 code shows that the factors of 10^3 and 10^6 associated with the terms involving WCONC(7,3,3) were missing from the original specifications. Equation (3.9.16) requires the sulphate concentration to be in [mol dm^{-3}]. WCONC(7,3,3) is in [mol m^{-3}]. (BWG, 87-03-30)

Figure 1.3.2.6B
Calculate CONC. TOTAL
TH DISS. MIXING LAYER
(THDISM)

THDISM - CONC. TOTAL TH DISS. MIXING LAYER [mol m^{-3}]. The concentration of total thorium (Th-230 and Th-232) that has dissolved in the mixing layer of the saturated zone to TIME=t.



Short Name	Long Name	SI Unit	Source
DMIX	THICKNESS OF MIXING ZONE	[m]	Sampled
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled
THDISM	CONC. TOTAL TH DISS. MIXING LAYER	[mol m^{-3}]	1.3.2.6B
THORCF	WT. TH CONVERS. FACTOR	[Bq mol^{-1}]	1.3.1.11
WCONC(2,2,3)	AQ. TH IN UNSAT. ZONE	[Bq m^{-3}]	1.3.2.4
WCONC(2,3,3)	AQ. TH IN MIXING LAYER	[Bq m^{-3}]	1.3.2.6A

(a) If WCONC(2,3,3) < WCONC(2,2,3) use the finite difference equation

$$\mathrm{THDISM}(t) = \mathrm{THDISM}(t-\Delta t) - \frac{\mathrm{NPRCP} * \mathrm{DT} * (\mathrm{WCONC}(2,2,3) - \mathrm{WCONC}(2,3,3))}{\mathrm{DMIX} * \mathrm{THORCF}} \qquad \text{(eqn. 3.9.17)}$$

(b) If WCONC(2,3,3) $\geq$ WCONC(2,2,3) use the finite difference equation

$$\mathrm{THDISM}(t) = \mathrm{THDISM}(t-\Delta t) + \frac{\mathrm{NPRCP} * \mathrm{DT} * \mathrm{WCONC}(2,3,3)}{\mathrm{DMIX} * \mathrm{THORCF}} \qquad \text{(eqn. 3.9.18)}$$

Unit check: (a and b)

$$[\mathrm{mol\ m}^{-3}] + \frac{[\mathrm{m\ a}^{-1}] * [\mathrm{a}] * [\mathrm{Bq\ m}^{-3}]}{[\mathrm{m}] * [\mathrm{Bq\ mol}^{-1}]} = [\mathrm{mol\ m}^{-3}]$$

Note 1: The factor THORCF is required to convert WCONC(2,2,3) and WCONC(2,3,3) from [Bq m^{-3}] to [mol m^{-3}].

Note 2: THDISM = 0.0 at TIME=-Δt (SENES letter 87-01-27).

Note 3: Inspection of the UTAP2 code shows that THDISM=0 at t=0. (BWG, 87-04-13)

Figure 1.3.2.7
Recalculate AQ. TH
IN MIXING LAYER
(WCONC(2,3,3))

WCONC(2,3,3) - AQ. TH IN MIXING LAYER [Bq m^{-3}]. The concentration of thorium in the aqueous phase in the mixing layer of the saturated zone.

THSOL - - -> WCONC(2,3,3) <—— WCONC(2,3,3)
THDISM

Short Name	Long Name	SI Unit	Source
THDISM	CONC. TOTAL TH DISS. MIXING LAYER	[mol m^{-3}]	1.3.2.6B
THSOL	INIT. CONC. TOTAL SOLU. TH	[mol m^{-3}]	1.3.1.8
WCONC(2,3,3)	AQ. TH IN MIXING LAYER	[Bq m^{-3}]	1.3.2.6A & 1.3.2.7

(a) If THDISM(t) $\geq$ THSOL

$$\mathrm{WCONC}(2,3,3) = 0 \qquad \text{(eqn. 3.9.19)}$$

(b) If THDISM(t) < THSOL

$$\mathrm{WCONC}(2,3,3) = \mathrm{WCONC}(2,3,3)$$

Unit check: [Bq m^{-3}] = [Bq m^{-3}]

Figure 1.3.2.8
Calculate AQ. TH IN
BOTTOM SAT. ZONE
(WCONC(2,4,3))

WCONC(2,4,3) - AQ. TH IN BOTTOM SAT. ZONE [Bq m^{-3}]. The concentration of thorium in the aqueous phase in the bottom layer of the saturated zone.

```
THORCF
FACTCO  - - ->  WCONC(2,4,3)  <——  PH4
THORDC                             WCONC(7,4,3)
```

Short Name	Long Name	SI Unit	Source
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
PH4	PH LAYER 4	[-]	1.1.5.5
THORCF	WT. TH CONVERS. FACTOR	[Bq mol^{-1}]	1.3.1.11
THORDC	LOG APPAR. SOL. PROD. $TH(OH)_4$	[-]	1.3.1.12
WCONC(2,4,3)	AQ. TH IN BOTTOM SAT. ZONE	[Bq m^{-3}]	1.3.2.8
WCONC(7,4,3)	CONC. OF SO_4 AQ. IN BOTTOM LAYER	[mol m^{-3}]	1.1.5.3

$$\mathrm{WCONC(2,4,3)} = \frac{1000. * \mathrm{THORCF} * 10^{(\mathrm{THORDC}-4*\mathrm{PH4})}}{(\mathrm{FACTCO})^{4.0}} * \Big\{ 1 + (\mathrm{FACTCO})^{1.75}$$

$$* 10^{(\mathrm{PH4}-3.2)} + (\mathrm{FACTCO})^{3} * 10^{(2*\mathrm{PH4}-6.93)} + (\mathrm{FACTCO})^{3.75} * 10^{(3*\mathrm{PH4}-11.7)}$$

$$+ (\mathrm{FACTCO})^{4} * 10^{(4*\mathrm{PH4}-15.9)} + (\mathrm{FACTCO})^{4} * 10^{5.45} * \mathrm{WCONC(7,4,3)} / 10^{3}$$

$$+ (\mathrm{FACTCO})^{6} * 10^{9.73} * \mathrm{WCONC(7,4,3)} * \mathrm{WCONC(7,4,3)} / 10^{6} \Big\} \quad \text{(eqn. 3.9.16)}$$

If $\mathrm{WCONC(2,4,3)} > 1000 * \mathrm{THORCF} * 5 * 10^{-5}$

$\mathrm{WCONC(2,4,3)} = 1000 * \mathrm{THORCF} * 5 * 10^{-5}$ (below eqn. 3.9.16)

Unit check: (see Note 3) [dm m^{-3}] * [Bq mol^{-1}] * [mol dm^{-3}] = [Bq m^{-3}]

Note 1: The factors 10^3 [dm^3 m^{-3}] and THORCF [Bq mol^{-1}] are necessary to obtain WCONC(2,4,3) in [Bq m^{-3}].

Note 2: The bottom layer is assumed to be large enough, and the chemical composition such that thorium depletion is not expected to occur over the 1000 year modelling period (SENES Vol. 3, pg 3-76).

Note 3: It is assumed the terms in brackets { } are dimensionless.

Note 4: The factors of 10^3 and 10^6 associated with the terms involving WCONC(7,4,3) were missing from the original specifications. Equation (3.9.16) requires the sulphate concentration in [mol dm^{-3}] while WCONC(7,4,3) is in [mol m^{-3}]. (BWG, 87-03-30)

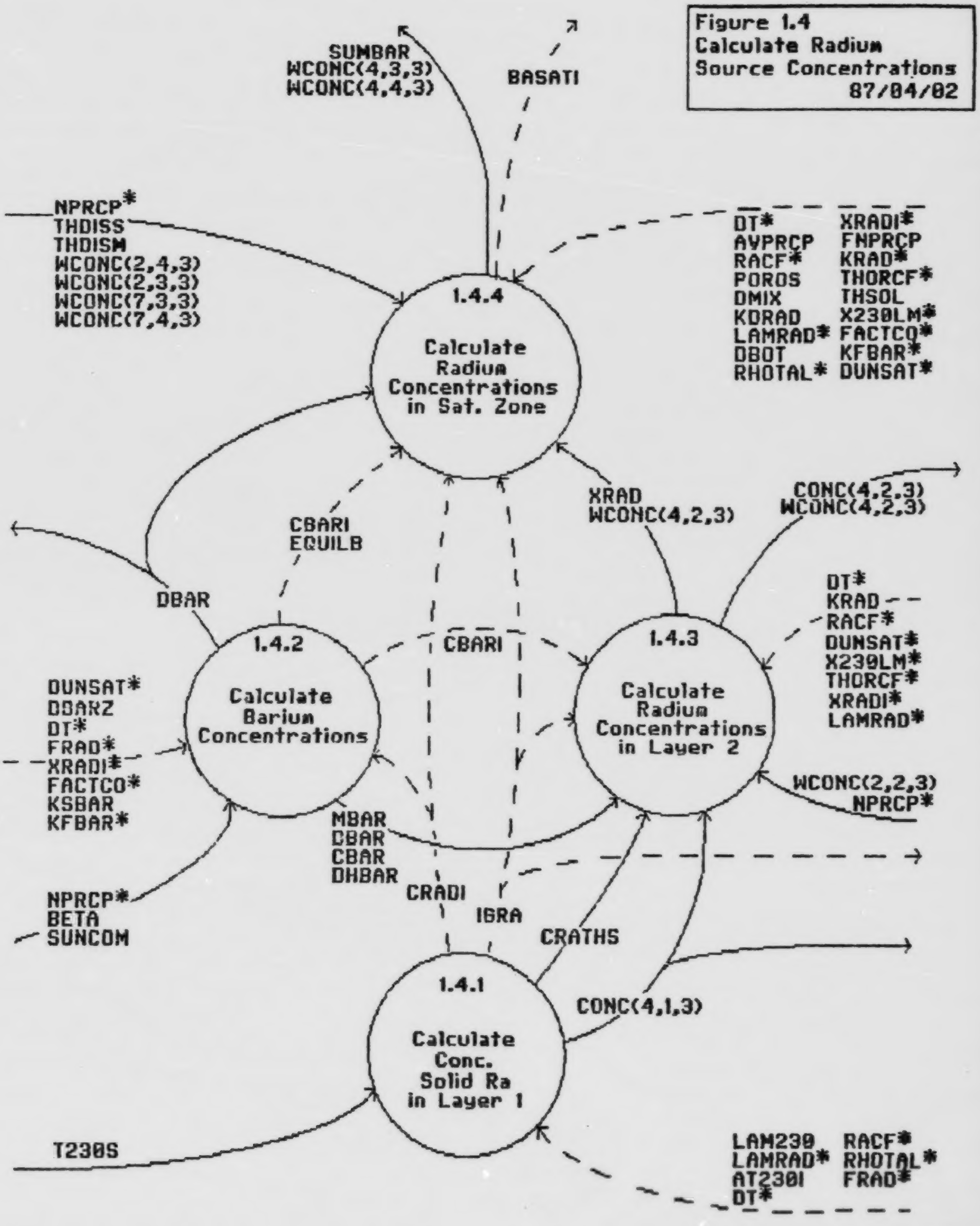
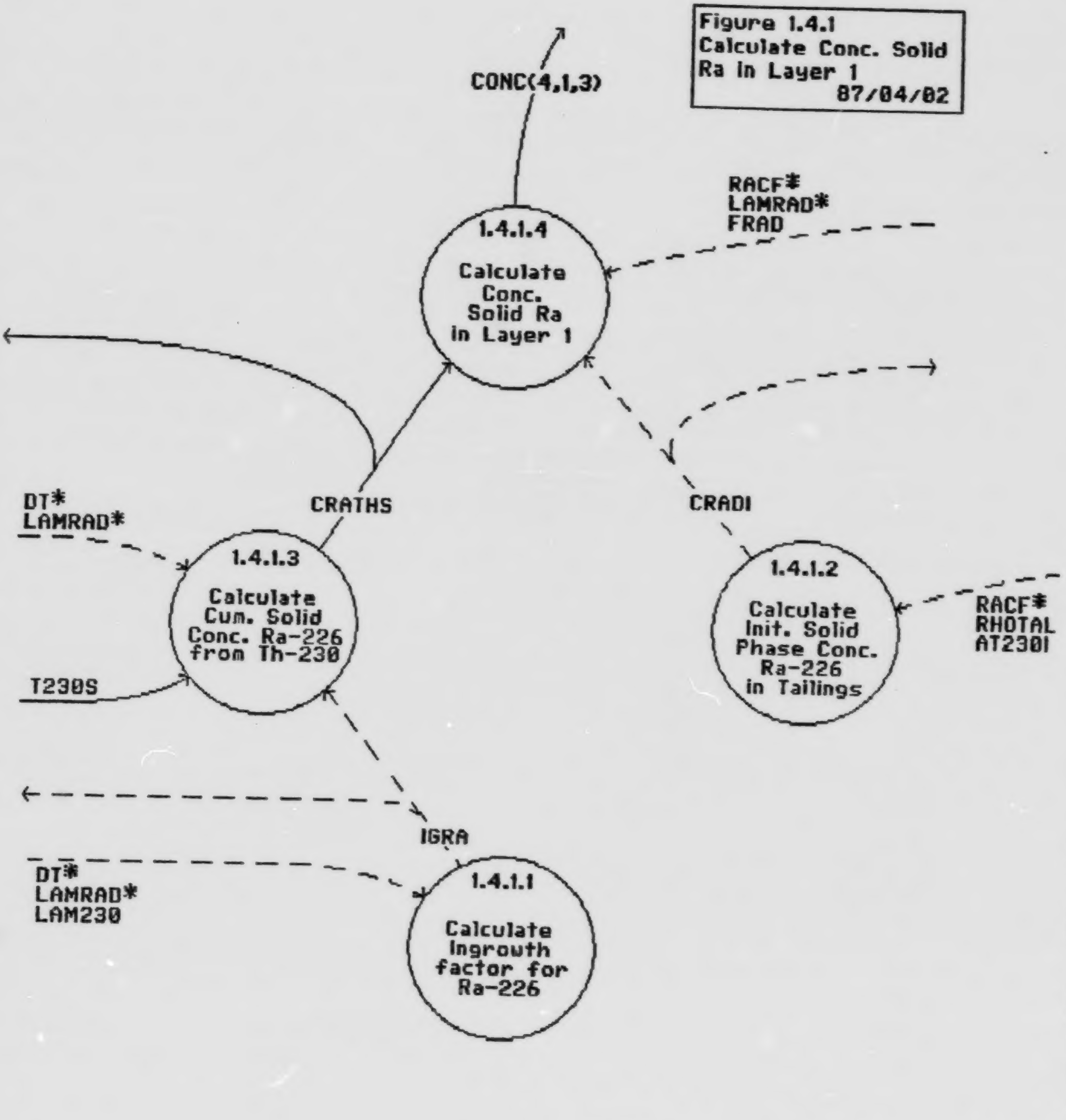

SUMBAR
WCONC(4,3,3)
WCONC(4,4,3)
BASATI
NPRCP*
THDISS
THDISM
WCONC(2,4,3)
WCONC(2,3,3)
WCONC(7,3,3)
WCONC(7,4,3)
DT*
AVPRCP
RACF*
POROS
DMIX
KDRAD
LAMRAD*
DBOT
RHOTAL*
XRADI*
FNPRCP
KRAD*
THORCF*
THSOL
X230LM*
FACTCO*
KFBAR*
DUNSAT*
1.4.4
Calculate
Radium
Concentrations
in Sat. Zone
XRAD
WCONC(4,2,3)
CONC(4,2,3)
WCONC(4,2,3)
CBARI
EQUILB
DBAR
DT*
KRAD
RACF*
DUNSAT*
X230LM*
THORCF*
XRADI*
LAMRAD*
1.4.2
Calculate
Barium
Concentrations
CBARI
1.4.3
Calculate
Radium
Concentrations
in Layer 2
DUNSAT*
DDARZ
DT*
FRAD*
XRADI*
FACTCO*
KSBAR
KFBAR*
WCONC(2,2,3)
NPRCP*
MBAR
CBAR
CBAR
DHBAR
CRADI
IGRA
CRATHS
NPRCP*
BETA
SUNCOM
1.4.1
Calculate
Conc.
Solid Ra
in Layer 1
CONC(4,1,3)
T230S
LAM230
LAMRAD*
AT230I
DT*
RACF*
RHOTAL*
FRAD*

Figure 1.4
Calculate Radium
Source Concentrations
87/04/02

Figure 1.4.1
Calculate Conc. Solid
Ra in Layer 1
87/04/02


CONC(4,1,3)
RACF*
LAMRAD*
FRAD
1.4.1.4
Calculate Conc. Solid Ra in Layer 1
CRATHS
CRADI
DT*
LAMRAD*
1.4.1.3
Calculate Cum. Solid Conc. Ra-226 from Th-230
T230S
1.4.1.2
Calculate Init. Solid Phase Conc. Ra-226 in Tailings
RACF*
RHOTAL
AT230I
IGRA
DT*
LAMRAD*
LAM230
1.4.1.1
Calculate Ingrowth factor for Ra-226

IGRA - INGROWTH FACTOR FOR RA-226 [-].
The factor used to approximate the ingrowth of Ra-226 from Th-230.

Figure 1.4.1.1
Calculate INGROWTH
FACTOR FOR RA-226
(IGRA)

LAM230
LAMRAD - - -> IGRA
DT≡Δt

Short Name	Long Name	SI Unit	Source
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
IGRA	INGROWTH FACTOR FOR RA-226	[-]	1.4.1.1
LAM230	TH-230 DECAY CONSTANT	$[a^{-1}]$	Sampled
LAMRAD	RA-226 DECAY CONSTANT	$[a^{-1}]$	Sampled

$$\mathrm{IGRA} = \left(\frac{\mathrm{LAM230}}{(\mathrm{LAMRAD} - \mathrm{LAM230})}\right) * \left[\mathrm{EXP}(-\mathrm{LAM230} * \mathrm{DT}) - \mathrm{EXP}(-\mathrm{LAMRAD} * \mathrm{DT})\right]$$

(portion SENES
eqn. 3.10.27)

Unit check:

$$\mathrm{IGRA} \left(\frac{[a^{-1}]}{([a^{-1}] - a^{-1}])}\right) * \left[\mathrm{EXP}\ ([a^{-1}] * [a])\ -\mathrm{EXP}\ ([a^{-1}] * [a])\right] = [-]$$

Note: This factor is not defined by SENES but was defined here for convenience. It is used in several equations in the TSOURC modules and elsewhere.

CRADI - INIT. SOLID PHASE CONC. RA-226 IN TAILINGS [mol m^{-3}]. The initial solid phase concentration of Ra-226 in the tailings.

Figure 1.4.1.2
Calculate INIT. SOLID PHASE CONC. RA-226 IN TAILINGS (CRADI)

```
ARADI
RHOTAL    - - ->   CRADI
RACF

AT230I    - - ->   ARADI
```

Short Name	Long Name	SI Unit	Source
ARADI	INIT. ACTIV. RA-226 IN TAILINGS	[Bq g^{-1}]	(1.4.1.2)
AT230I	INIT. ACTIV. TH-230 IN TAILINGS	[Bq g^{-1}]	1.3.1.1
CRADI	INIT. SOLID PHASE CONC. RA-226 IN TAILINGS	[mol m^{-3}]	1.4.1.2
RACF	CONVERSION FACTOR MOL TO BQ (RA-226)	[Bq mol^{-1}]	Sampled
RHOTAL	TAILINGS BULK DENSITY	[g m^{-3}]	Sampled

CRADI = ARADI * RHOTAL / RACF (eqn. 3.7.35)

ARADI = AT230I (eqn. 3.7.33)

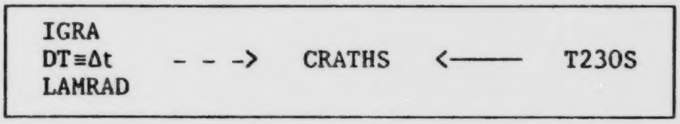
Unit check:

CRADI [Bq g^{-1}] * [g m^{-3}] / [Bq mol^{-1}] = [mol m^{-3}]

ARADI [Bq g^{-1}] = [Bq g^{-1}]

CRATHS - CUM. SOLID CONC. RA-226 FROM TH-230 [mol m^{-3}]. The cumulative solid phase concentration of Ra-226 resulting from ingrowth from Th-230 to TIME=t.

Figure 1.4.1.3
Calculate CUM. SOLID CONC. RA-226 FROM TH-230



Short Name	Long Name	SI Unit	Source
CRATHS	CUM. SOLID CONC. RA-226 FROM TH-230	[mol m^{-3}]	1.4.1.3
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
IGRA	INGROWTH FACTOR FOR RA-226	[-]	1.4.1.1
LAMRAD	RA-226 DECAY CONSTANT	[a^{-1}]	Sampled
T230S	CONC. SOLID TH-230 IN UNSAT. ZONE	[mol m^{-3}]	1.3.2.3

Solve the following finite difference equation for CRATHS

$$\text{CRATHS}(t) = (\text{CRATHS}(t-\Delta t)) * \text{EXP}(-\text{DT} * \text{LAMRAD}) + \text{T230S} * \text{IGRA} \qquad \text{(eqn. 3.10.23)}$$

Unit check:

CRATHS EXP: [a] x [a^{-1}] = [-]

CRATHS: [mol m^{-3}] * [-] + [mol m^{-3}] * [-] = [mol m^{-3}]

Note 1: The first exponential of equation (3.10.23) should read ($-\lambda_{Ra-226}$ Δt) (SENES letter 1986-12-02).

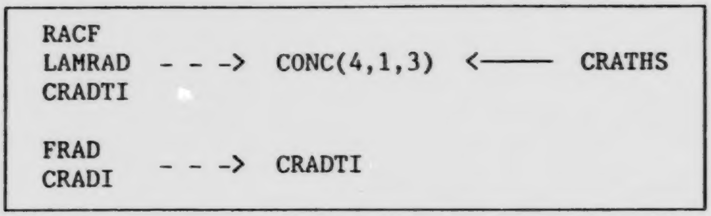
Note 2: Equation (3.10.23) has been modified (simplified) by use of our defined factor IGRA (see Figure 1.4.1.1).

Note 3: It is assumed CRATHS(-Δt) is zero (SENES letter 1987-01-27).

Note 4: Inspection of the UTAP2 code shows that CRATHS(0)=0 (as well as, apparently, at t=-Δt). (BWG, 87-04-02)

CONC(4,1,3) - CONC. SOLID RA IN LAYER 1 ([Bq m^{-3}]. Solid phase concentration of radium in the upper layer of the unsaturated zone.

Figure 1.4.1.4
Calculate CONC. SOLID RA IN LAYER 1 (CONC(4,1,3))



Short Name	Long Name	SI Unit	Source
CONC(4,1,3)	CONC. SOLID RA IN LAYER 1	[Bq m^{-3}]	1.4.1.4
CRADI	INIT. SOLID PHASE CONC. RA-226 IN TAILINGS	[mol m^{-3}]	1.4.1.2
CRADTI	INIT. CONC. RA-226 ASSOC. WITH HOST TAILINGS	[mol m^{-3}]	(1.4.1.4)
CRATHS	CUM. SOLID CONC. RA-226 FROM TH-230	[mol m^{-3}]	1.4.1.3
FRAD	FRACT. RA SOLUBLE	[-]	Sampled
LAMRAD	RA-226 DECAY CONSTANT	[a^{-1}]	Sampled
RACF	CONVERSION FACTOR MOL TO BQ (RA-226)	[Bq mol^{-1}]	Sampled

If t=0 then CONC(4,1,3) = CRADTI * RACF (see Note 2)

If t>0

CRADTI = (1 - FRAD) * CRADI (eqn. 3.7.37)

CONC(4,1,3) = (CRATHS(t) + CRADTI * EXP(-LAMRAD * TIME)) * RACF (eqn. 3.10.24)

Unit check:

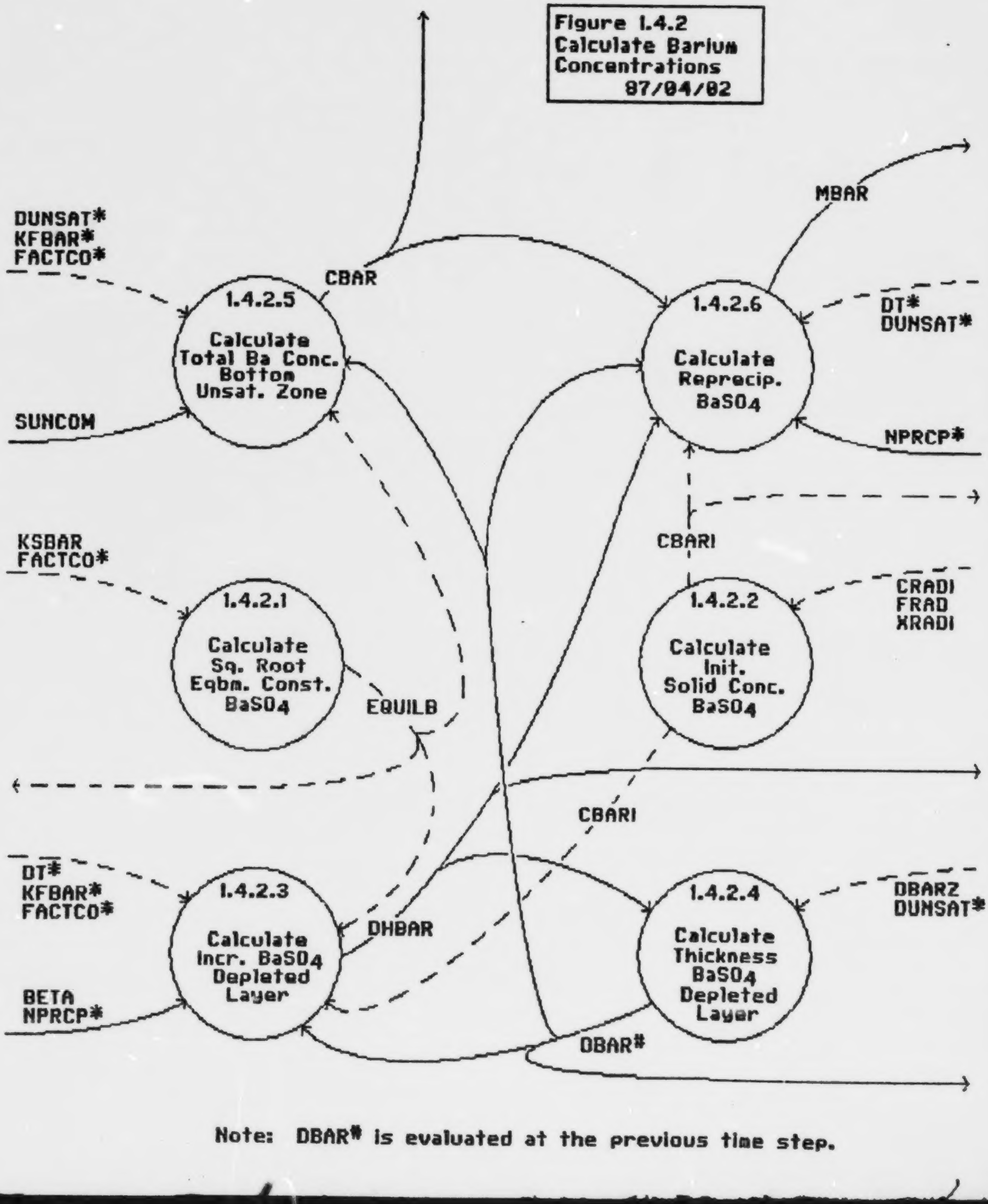
CRADTI: [-] * [mol m^{-3}] = [mol m^{-3}]

CONC(4,1,3): ([mol m^{-3}] + [mol m^{-3}] * EXP([a^{-1}] * [a])) * [Bq mol^{-1}] = [Bq m^{-3}]

Note 1: The factor RACF has been used to maintain consistent units for CONC(4,1,3) of [Bq m^{-3}].

Note 2: The initial condition for CONC(4,1,3) is based on an examination of the UTAP2 code. (BWG, 87-04-01)

Figure 1.4.2
Calculate Barium
Concentrations
87/04/02


CBAR
MBAR
DUNSAT*
KFBAR*
FACTCO*
1.4.2.5
Calculate
Total Ba Conc.
Bottom
Unsat. Zone
SUNCOM
1.4.2.6
Calculate
Reprecip.
BaSO4
DT*
DUNSAT*
NPRCP*
CBARI
KSBAR
FACTCO*
1.4.2.1
Calculate
Sq. Root
Eqbm. Const.
BaSO4
EQUILB
1.4.2.2
Calculate
Init.
Solid Conc.
BaSO4
CRADI
FRAD
XRADI
CBARI
DT*
KFBAR*
FACTCO*
1.4.2.3
Calculate
Incr. BaSO4
Depleted
Layer
DHBAR
BETA
NPRCP*
1.4.2.4
Calculate
Thickness
BaSO4
Depleted
Layer
DBARZ
DUNSAT*
DBAR#

Note: DBAR# is evaluated at the previous time step.

Figure 1.4.2.1
Calculate SQ. ROOT
EQBM. CONST. $BaSO_4$
(EQUILB)

EQUILB - SQ. ROOT EQBM. CONST. $BaSO_4$ [mol m^{-3}]
EQUILB is an intermediate variable, equal to the square root of the solubility product for barium sulphate, divided by the activity coefficient.

$$\begin{matrix} \text{KSBAR} \\ \text{FACTCO} \end{matrix} \dashrightarrow \text{EQUILB}$$

Short Name	Long Name	SI Unit	Source
EQUILB	SQ. ROOT EQBM. CONST. $BASO_4$	[mol m^{-3}]	1.4.2.1
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
KSBAR	SOLUBILITY EQM. CONST. FOR $BASO_4$	[mol^2 m^{-6}]	Sampled

$$\text{EQUILB} = \sqrt{\frac{\text{KSBAR}}{(\text{FACTCO})^2}} \qquad \text{(near eqn. 3.10.6)}$$

Unit check: $\left(\frac{[mol^2\ m^{-6}]}{[-]^2}\right)^{0.5} = [mol\ m^{-3}]$

Note 1: Symbol "a" is in the text but EQUILB is not defined in Table A.3.

Note 2: The value of KSBAR in Table A.3 is incorrect (SENES letter 1986-11-04). The value on page 3-78 should be used.

CBARI - INIT. SOLID CONC. $BASO_4$ [mol m^{-3}]. The initial solid phase concentration of barium sulphate in the tailings.

Figure 1.4.2.2
Calculate INIT. SOLID
CONC. $BASO_4$
(CBARI)

FRAD
XRADI - - -> CBARI
CRADI

Short Name	Long Name	SI Unit	Source
CBARI	INIT. SOLID CONC. $BASO_4$	[mol m^{-3}]	1.4.2.2
CRADI	INIT. SOLID PHASE CONC. RA-226 IN TAILINGS	[mol m^{-3}]	1.4.1.2
FRAD	FRACT. RA SOLUBLE	[-]	Sampled
XRADI	INIT. MOLE FRACT. RA-226	[-]	Sampled

$$\text{CBARI} = \frac{\text{FRAD} * \text{CRADI}}{\text{XRADI}}$$ (eqns. 3.7.36 and 3.7.38)

Unit check:

$$\frac{[-] * [\text{mol m}^{-3}]}{[-]} = [\text{mol m}^{-3}]$$

Figure 1.4.2.3
Calculate INCR. $BASO_4$
DEPLETED LAYER
(DHBAR)

DHBAR - INCR. $BASO_4$ DEPLETED LAYER [m].
Increase in the thickness of the barium sulphate depleted layer over the time interval Δt.

FACTCO
EQUILB
KFBAR - - -> DHBAR <—— DBAR(t-Δt), BETA, NPRCP
CBARI
DT≡Δt

Short Name	Long Name	SI Unit	Source
BETA	PYRITE OXIDATION FACTOR	$[\mathrm{mol\ m^{-3}}]$	1.1.2.4
CBARI	INIT. SOLID CONC. $BASO_4$	$[\mathrm{mol\ m^{-3}}]$	1.4.2.2
DBAR	THICKNESS $BASO_4$ DEPLETED LAYER	[m]	1.4.2.4
DHBAR	INCR. $BASO_4$ DEPLETED LAYER	[m]	1.4.2.3
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
EQUILB	SQ. ROOT EQBM. CONST. $BASO_4$	$[\mathrm{mol\ m^{-3}}]$	1.4.2.1
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
KFBAR	$BASO_4$ FORMATION CONSTANT	$[\mathrm{m^3\ mol^{-1}}]$	Sampled
NPRCP	NET PRECIPITATION	$[\mathrm{m\ a^{-1}}]$	Sampled

$$\mathrm{DHBAR} = \left\{ \frac{(\mathrm{EQUILB})^2 * \mathrm{NPRCP} * \mathrm{DT}}{\mathrm{CBARI}} * \left[\frac{\mathrm{NPRCP} * \mathrm{DT}}{\mathrm{BETA}} + 2 * (\mathrm{FACTCO})^2 * \mathrm{KFBAR} * \mathrm{DBAR}(t-\Delta t) \right] \right.$$

$$\left. + \frac{1}{4} * \left[2 * \mathrm{DBAR}(t-\Delta t) + \frac{\mathrm{EQUILB} * \mathrm{NPRCP} * \mathrm{DT}}{\mathrm{BETA}} - \frac{(\mathrm{EQUILB})^2 * (\mathrm{FACTCO})^2 * \mathrm{KFBAR} * \mathrm{NPRCP} * \mathrm{DT}}{\mathrm{CBARI}} \right]^2 \right\}^{0.5}$$

$$- \left[\mathrm{DBAR}(t-\Delta t) + \frac{\mathrm{EQUILB} * \mathrm{NPRCP} * \mathrm{DT}}{2 * \mathrm{BETA}} - \frac{(\mathrm{EQUILB})^2 * (\mathrm{FACTCO})^2 * \mathrm{KFBAR} * \mathrm{NPRCP} * \mathrm{DT}}{2 * \mathrm{CBARI}} \right]$$

(eqn. 3.10.6)

Unit check:

$$\left\{ \frac{[\mathrm{mol\ m^{-3}}]^2 * [\mathrm{m\ a^{-1}}] * [\mathrm{a}]}{[\mathrm{mol\ m^{-3}}]} * \left[\frac{[\mathrm{m\ a^{-1}}] * [\mathrm{a}]}{[\mathrm{mol\ m^{-3}}]} + [-]^2 * [\mathrm{m^3\ mol^{-1}}] * [\mathrm{m}] \right] \right.$$

$$\left. + \left[[\mathrm{m}] + \frac{[\mathrm{mol\ m^{-3}}] * [\mathrm{m\ a^{-1}}] * [\mathrm{a}]}{[\mathrm{mol\ m^{-3}}]} - \frac{[\mathrm{mol\ m^{-3}}] * [-]^2 * [\mathrm{m^3\ mol^{-1}}] * [\mathrm{m\ a^{-1}}] * [\mathrm{a}]}{[\mathrm{mol\ m^{-3}}]} \right]^2 \right\}^{0.5}$$

$$- \left[[\mathrm{m}] + \frac{[\mathrm{mol\ m^{-3}}] * [\mathrm{m\ a^{-1}}] * [\mathrm{a}]}{[\mathrm{mol\ m^{-3}}]} - \frac{[\mathrm{mol\ m^{-3}}]^2 * [-] * [\mathrm{m^3\ mol^{-1}}] * [\mathrm{m\ a^{-1}}] * [\mathrm{a}]}{[\mathrm{mol\ m^{-3}}]} \right] = [\mathrm{m}]$$

Note: DHBAR is not calculated between TIME t=-Δt and TIME=0. DBAR(TIME=0) is 0.01[m]. See SENES Vol. 3 pg. 3-81.

Figure 1.4.2.4
Calculate THICKNESS
$BASO_4$ DEPLETED LAYER
(DBAR)

DBAR - THICKNESS $BASO_4$ DEPLETED LAYER [m]. The thickness of the barium sulphate depleted layer of the tailings.

$$\begin{tikzcd} \begin{array}{l}\text{DBARZ}\\ \text{DUNSAT}\end{array} \arrow[r, dashed] & \text{DBAR}(t) & \begin{array}{l}\text{DBAR}(t-\Delta t)\\ \text{DHBAR}\end{array} \arrow[l] \end{tikzcd}$$

Short Name	Long Name	SI Unit	Source
DBAR	THCKNESS $BaSO_4$ DEPLETED LAYER	[m]	1.4.2.4
DBARZ	THICKNESS OF $BaSO_4$ DEPLETED LAYER AT TIME=0	[m]	Sampled
DHBAR	INCR. $BaSO_4$ DEPLETED LAYER	[m]	1.4.2.3
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled

If TIME = $-\Delta t$
DBAR = 0.0 (SENES pg. 3-81;

If TIME = 0.0
DBAR = DBARZ (SENES pg. 3-81)

If TIME = < 0.0 from the finite difference equation
DBAR(t) = DBAR(t-Δt) + DHBAR (below eqn. 3.10.6)

If (DBAR $\geq$ DUNSAT) then
DBAR = DUNSAT

Unit check:
DBAR: [m] + [m] = [m]

Note 1: Inspection of the UTAP2 code shows that, if DBAR $\geq$ DUNSAT, it is reset to equal DUNSAT. (BWG, 87-05-07)

Figure 1.4.2.5
Calculate TOTAL BA CONC. BOTTOM UNSAT. ZONE (CBAR)

CBAR - TOTAL BA CONC. BOTTOM UNSAT. ZONE [mol m^{-3}]. Total concentration of dissolved barium at the bottom of the unsaturated zone.

EQUILB
KFBAR
FACTCO
DUNSAT
- - -> CBAR <—— DBAR
SUNCOM

Short Name	Long Name	SI Unit	Source
CBAR	TOTAL BA CONC. BOTTOM UNSAT. ZONE	[mol m^{-3}]	1.4.2.5
DBAR	THICKNESS $BASO_4$ DEPLETED LAYER	[m]	1.4.2.4
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
EQUILB	SQ. ROOT EQBM. CONST. $BASO_4$	[mol m^{-3}]	1.4.2.1
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
KFBAR	$BASO_4$ FORMATION CONSTANT	[m^3 mol^{-1}]	Sampled
SUNCOM	CONC. UNCOMP. SO_4 BOTTOM UNSAT. ZONE	[mol dm^{-3}]	1.1.2.12

$$\text{CBAR} = \left(\frac{\text{EQUILB} * \text{EQUILB}}{\text{EQUILB} + \text{SUNCOM} * 1000}\right) * \left(1 + (\text{FACTCO})^2 * \text{KFBAR} * \text{SUNCOM} * 1000\right)$$

(eqn. 3.10.9)

If DBAR $\geq$ DUNSAT then
CBAR = 0

Unit check:

$$\text{CBAR:} \quad \frac{[\text{mol m}^{-3}]^2}{[\text{mol m}^{-3}] + [\text{mol dm}^{-3}] * [\text{dm}^3\ \text{m}^{-3}]} *$$

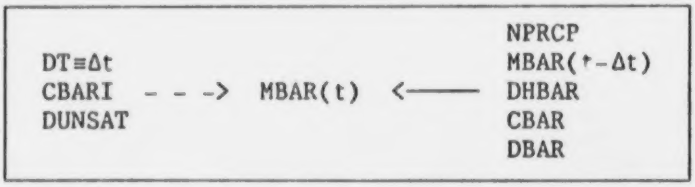
$$\left(1 + [-]^2 * [\text{m}^3\ \text{mol}^{-1}] * [\text{mol dm}^{-3}] * [\text{dm}^3\ \text{m}^{-3}]\right) = [\text{mol m}^{-3}]$$

Note 1: The factors of 1000 [dm^3 m^{-3}] are required to express the concentration of uncomplexed sulphate correctly in [mol m^{-3}]. Equation (3.10.9) has been further modified (simplified) by use of the expression EQUILB defined by an equation below equation (3.10.6).

Note 2: Inspection of the UTAP2 code shows that, if DBAR $\geq$ DUNSAT, CBAR is reset to zero. (BWG, 87-05-07)

Figure 1.4.2.6
Calculate REPRECIP.
$BASO_4$
(MBAR)

MBAR - REPRECIP. BASO4 [mol m^{-2}].
The amount of barite ($BaSO_4$) reprecipitated in the unsaturated zone (per unit area).



Short Name	Long Name	SI Unit	Source
CBAR	TOTAL BA CONC. BOTTOM UNSAT. ZONE	[mol m^{-3}]	1.4.2.5
CBARI	INIT. SOLID CONC. $BASO_4$	[mol m^{-3}]	1.4.2.2
DBAR	THICKNESS $BASO_4$ DEPLETED LAYER	[m]	1.4.2.4
DHBAR	INCR. $BASO_4$ DEPLETED LAYER	[m]	1.4.2.3
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
MBAR	REPRECIP. $BASO_4$	[mol m^{-2}]	1.4.2.6
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled

Calculated from the finite difference equation

$$MBAR(t) = MBAR(t-\Delta t) + CBARI * DHBAR - NPRCP * DT * CBAR$$

(eqn. 3.10.11)

If DBAR $\geq$ DUNSAT then
MBAR = 0

Unit check:

$$[mol\ m^{-2}] + [mol\ m^{-3}] * [m] - [m\ a^{-1}] * [a] * [mol\ m^{-3}] = [mol\ m^{-2}]$$

Note 1: Equation assumed valid for t>0. MBAR is assumed to be zero at t=0.

Note 2: Inspection of the UTAP2 code shows that, if DBAR $\geq$ DUNSAT, MBAR is reset to 0. (BWG, 87-05-07)

Figure 1.4.3
Calculate Radium
Concentrations in Layer 2
87/04/03

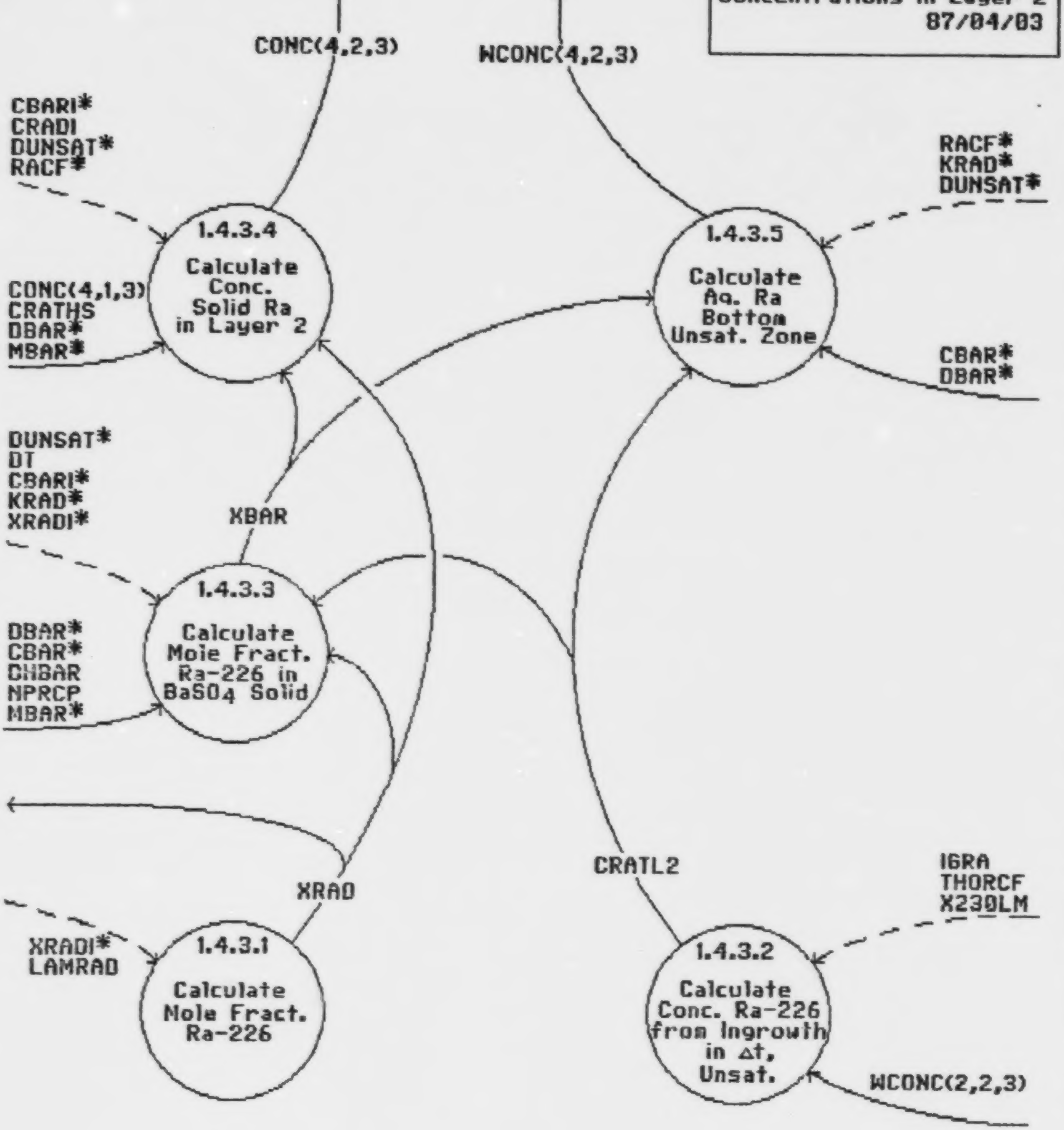

CONC(4,2,3)
WCONC(4,2,3)
CBARI*
CRADI
DUNSAT*
RACF*
RACF*
KRAD*
DUNSAT*
1.4.3.4
Calculate
Conc.
Solid Ra
in Layer 2
1.4.3.5
Calculate
Aq. Ra
Bottom
Unsat. Zone
CONC(4,1,3)
CRATHS
DBAR*
MBAR*
CBAR*
DBAR*
DUNSAT*
DT
CBARI*
KRAD*
XRADI*
XBAR
1.4.3.3
Calculate
Mole Fract.
Ra-226 in
BaSO4 Solid
DBAR*
CBAR*
DHBAR
NPRCP
MBAR*
XRAD
CRATL2
IGRA
THORCF
X230LM
XRADI*
LAMRAD
1.4.3.1
Calculate
Mole Fract.
Ra-226
1.4.3.2
Calculate
Conc. Ra-226
from Ingrowth
in Δt,
Unsat.
WCONC(2,2,3)

Figure 1.4.3.1
Calculate MOLE FRACT.
RA-226
(XRAD)

XRAD - MOLE FRACT. RA-226 [-].
Mole fraction of $^{226}RaSO_4$ in the barium sulphate, corrected for decay of Ra-226.

LAMRAD
XRADI
- - -> XRAD

Short Name	Long Name	SI Unit	Source
LAMRAD	RA-226 DECAY CONSTANT	$[a^{-1}]$	Sampled
XRAD	MOLE FRACT. RA-226	[-]	1.4.3.1
XRADI	INIT. MOLE FRACT. RA-226	[-]	Sampled

XRAD = XRADI * EXP(-LAMRAD * TIME) (eqn. 3.10.19)

Unit check:

XRAD: [-] * [-] = [-]

EXP: $[a^{-1}] * [a] = [-]$

Figure 1.4.3.2
Calculate CONC. RA-226
FROM INGROWTH IN Δt,
UNSAT. (CRATL2)

CRATL2 - CONC. RA-226 FROM INGROWTH IN Δt, UNSAT. [mol m^{-3}]. The concentration of Ra-226 at the bottom of the unsaturated zone resulting from ingrowth from Th-230 during the time step Δt.

X230LM
IGRA - - -> CRATL2 <—— WCONC(2,2,3)
THORCF

Short Name	Long Name	SI Unit	Source
CRATL2	CONC. RA-226 FROM INGROWTH IN Δt, UNSAT.	[mol m^{-3}]	1.4.3.2
IGRA	INGROWTH FACTOR FOR RA-226	[-]	1.4.1.1
THORCF	WT. TH CONVERS. FACTOR	[Bq mol^{-1}]	1.3.1.11
WCONC(2,2,3)	AQ. TH IN UNSAT. ZONE	[Bq m^{-3}]	1.3.2.4
X230LM	MOLE FRACT. TH-230	[-]	1.3.1.9

$$\text{CRATL2} = \frac{\text{X230LM} * \text{WCONC(2,2,3)} * \text{IGRA}}{\text{THORCF}}$$

(eqn. 3.10.20)

Unit check:

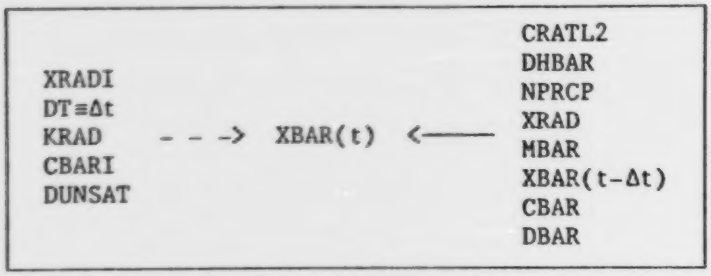
$$\text{CRATL2} \quad \frac{[-] * [\text{Bq m}^{-3}]}{[\text{Bq mol}^{-1}]} * [-] = [\text{mol m}^{-3}]$$

Note 1: The factor THORCF is necessary to give the liquid phase concentration of thorium at the bottom of the unsaturated layer in units of [mol m^{-3}] as WCONC(2,2,3) is in [Bq m^{-3}].

Note 2: Equation (3.10.20) has also been modified (simplified) by use of our defined factor IGRA (see Figure 1.4.1.1).

Figure 1.4.3.3
Calculate MOLE FRACT. RA-226 IN $BASO_4$ SOLID (XBAR)

XBAR - MOLE FRACT. RA-226 IN $BASO_4$ SOLID [-].
The solid phase mole fraction of Ra-226 in $BaSO_4$ at TIME=t.



Short Name	Long Name	SI Unit	Source
CBAR	TOTAL BA CONC. BOTTOM UNSAT. ZONE	$[mol\ m^{-3}]$	1.4.2.5
CBARI	INIT. SOLID CONC. $BASO_4$	$[mol\ m^{-3}]$	1.4.2.2
CRATL2	CONC. RA-226 FROM INGROWTH IN Δt, UNSAT.	$[mol\ m^{-3}]$	1.4.3.2
DBAR	THICKNESS OF $BASO_4$ DEPLETED LAYER	[m]	1.4.2.4
DHBAR	INCR. $BASO_4$ DEPLETED LAYER	[m]	1.4.2.3
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
KRAD	RA SOLID/AQ. DIST. COEFFICIENT	[-]	1.4.3.1
MBAR	REPRECIP. $BASO_4$	$[mol\ m^{-2}]$	1.4.2.6
NPRCP	NET PRECIPITATION	$[m\ a^{-1}]$	Sampled
XBAR	MOLE FRACT. RA-226 IN $BASO_4$ SOLID	[-]	1.4.3.3
XRAD	MOLE FRACT. RA-226	[-]	1.4.3.1
XRADI	INIT. MOLE FRACT. RA-226	[-]	Sampled

a) If t = 0 XBAR = XRADI (above eqn. 3.10.21)

b) If t > 0 from the finite difference equation

$$XBAR(t) = \frac{\left\{\begin{array}{r} CBARI * XRAD * DHBAR + NPRCP * CRATL2 * DT + MBAR(t-\Delta t) * XBAR(t-\Delta t) \\ - NPRCP * DT * CBAR * KRAD * XBAR(t-\Delta t) * 0.5 \end{array}\right\}}{MBAR(t) + NPRCP * DT * CBAR * KRAD * 0.5}$$

(eqn. 3.10.18;
see Note)

Unit check:

(a) [-] = [-]

$$\text{(b)}\quad \frac{\left\{\begin{array}{r} [mol\ m^{-3}] * [-] * [m] + [m\ a^{-1}] * [mol\ m^{-3}] * [a] + [mol\ m^{-2}] \\ * [-] - [m\ a^{-1}] * [a] * [mol\ m^{-3}] * [-] * [-] \end{array}\right\}}{[mol\ m^{-2}] + [m\ a^{-1}] * [a] * [mol\ m^{-3}] * [-]} = [-]$$

Note: Inspection of the UTAP2 code shows that this equation is used only when DBAR < DUNSAT; otherwise the denominator is zero. (BWG, 87-05-08)

CONC(4,2,3) - CONC. SOLID RA IN LAYER 2 [Bq m^{-3}]. Solid phase concentration of radium in the lower layer of the unsaturated zone.

Figure 1.4.3.4
Calculate CONC. SOLID RA IN LAYER 2 (CONC(4,2,3))

$$\begin{array}{ccccc} & & & & \text{CRATHS} \\ \text{CRADI} & & & & \text{DBAR} \\ \text{RACF} & \text{- - ->} & \text{CONC(4,2,3)} & \longleftarrow & \text{XRAD} \\ \text{CBARI} & & & & \text{MBAR} \\ \text{DUNSAT} & & & & \text{XBAR} \\ & & & & \text{CONC(4,1,3)} \end{array}$$

Short Name	Long Name	SI Unit	Source
CBARI	INIT. SOLID CONC. $BASO_4$	[mol m^{-3}]	1.4.2.2
CONC(4,1,3)	CONC. SOLID RA IN LAYER 1	[Bq m^{-3}]	1.4.1.4
CONC(4,2,3)	CONC. SOLID RA IN LAYER 2	[Bq m^{-3}]	1.4.3.4
CRADI	INIT. SOLID PHASE CONC. RA-226 IN TAILINGS	[mol m^{-3}]	1.4.1.2
CRATHS	CUM. SOLID CONC. RA-226 FROM TH-230	[mol m^{-3}]	1.4.1.3
DBAR	THICKNESS $BASO_4$ DEPLETED LAYER	[m]	1.4.2.4
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
MBAR	REPRECIP. $BASO_4$	[mol m^{-2}]	1.4.2.6
RACF	CONVERSION FACTOR MOL TO BQ (RA-226)	[Bq mol^{-1}]	Sampled
XBAR	MOLE FRACT. RA-226 IN $BASO_4$ SOLID	[-]	1.4.3.3
XRAD	MOLE FRACT. RA-226	[-]	1.4.3.1

If t = 0 then CONC(4,2,3) = CRADI * RACF (see Note 2)

Otherwise:
If DBAR < DUNSAT

$$\text{CONC(4,2,3)} = \left[\text{CRATHS(t)} + \text{XRAD} * \text{CBARI} + \frac{\text{XBAR} * \text{MBAR}}{(\text{DUNSAT} - \text{DBAR})}\right] * \text{RACF}$$

(eqn. 3.10.25)

If DBAR $\geq$ DUNSAT

CONC(4,2,3) = CONC(4,1,3) (below eqn. 3.10.25)

Unit check:

$$\left([\text{mol m}^{-3}] + [-] * [\text{mol m}^{-3}] + \left(\frac{[-] * [\text{mol m}^{-2}]}{[\text{m}] - [\text{m}]}\right)\right) * [\text{Bq mol}^{-1}] = [\text{Bq m}^{-3}]$$

Note 1: The factor RACF is required to convert the radium concentration from [mol m^{-3}] to CONC(4,2,3) in [Bq m^{-3}].

Note 2: The initial condition for CONC(4,2,3) is based on an examination of the UTAP2 code. (BWG, 87-04-01)

Note 3: Second term of eqn. (3.10.25) is read as $X'_{Ra/BaSO4}[BaSO_4]^{\circ}$.

WCONC(4,2,3) - AQ. RA BOTTOM UNSAT. ZONE [Bq m^{-3}]. The concentration of radium-226 in the aqueous phase at the bottom of the unsaturated zone.

Figure 1.4.3.5
Calculate AQ. RA BOTTOM UNSAT. ZONE (WCONC(4,2,3))

$$\begin{tikzcd} \begin{matrix}\text{RACF}\\ \text{KRAD}\\ \text{DUNSAT}\end{matrix} \arrow[r, dashed] & \text{WCONC(4,2,3)} & \begin{matrix}\text{DBAR}\\ \text{XBAR}\\ \text{CBAR}\\ \text{CRATL2}\end{matrix} \arrow[l] \end{tikzcd}$$

Short Name	Long Name	SI Unit	Source
CBAR	TOTAL BA CONC. BOTTOM UNSAT. ZONE	[mol m^{-3}]	1.4.2.5
CRATL2	CONC. RA-226 FROM INGROWTH IN Δt, UNSAT.	[mol m^{-3}]	1.4.3.2
DBAR	THICKNESS OF $BASO_4$ DEPLETED LAYER	[m]	1.4.2.4
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
KRAD	RA SOLID/AQ DIST. COEFFICIENT	[-]	Sampled
RACF	CONVERSION FACTOR MOL TO BQ (RA-226)	[Bq mol^{-1}]	Sampled
WCONC(4,2,3)	AQ. RA BOTTOM UNSAT. ZONE	[Bq m^{-3}]	1.4.3.5
XBAR	MOLE FRACT. RA-226 IN $BASO_4$ SOLID	[-]	1.4.3.3

(a) If DBAR < DUNSAT or if t = 0 (see Note 2)

WCONC(4,2,3) = KRAD * CBAR * XBAR * RACF (eqn. 3.10.21)

(b) If DBAR $\geq$ DUNSAT

WCONC(4,2,3) = CRATL2 * RACF (eqn. 3.10.22)

Unit check:

(a) [-] * [mol m^{-3}] * [-] * [Bq mol^{-1}] = [Bq m^{-3}]

(b) [mol m^{-3}] * [Bq mol^{-1}] = [Bq m^{-3}]

Note 1: The factor RACF [Bq mol^{-1}] is needed to convert the radium concentration to [Bq m^{-3}] (as in SENES Vol. 3 near the bottom of page 3-84).

Note 2: The initial condition for WCONC(4,2,3) was taken from inspection of the UTAP2 code. (BWG, 87-04-02)

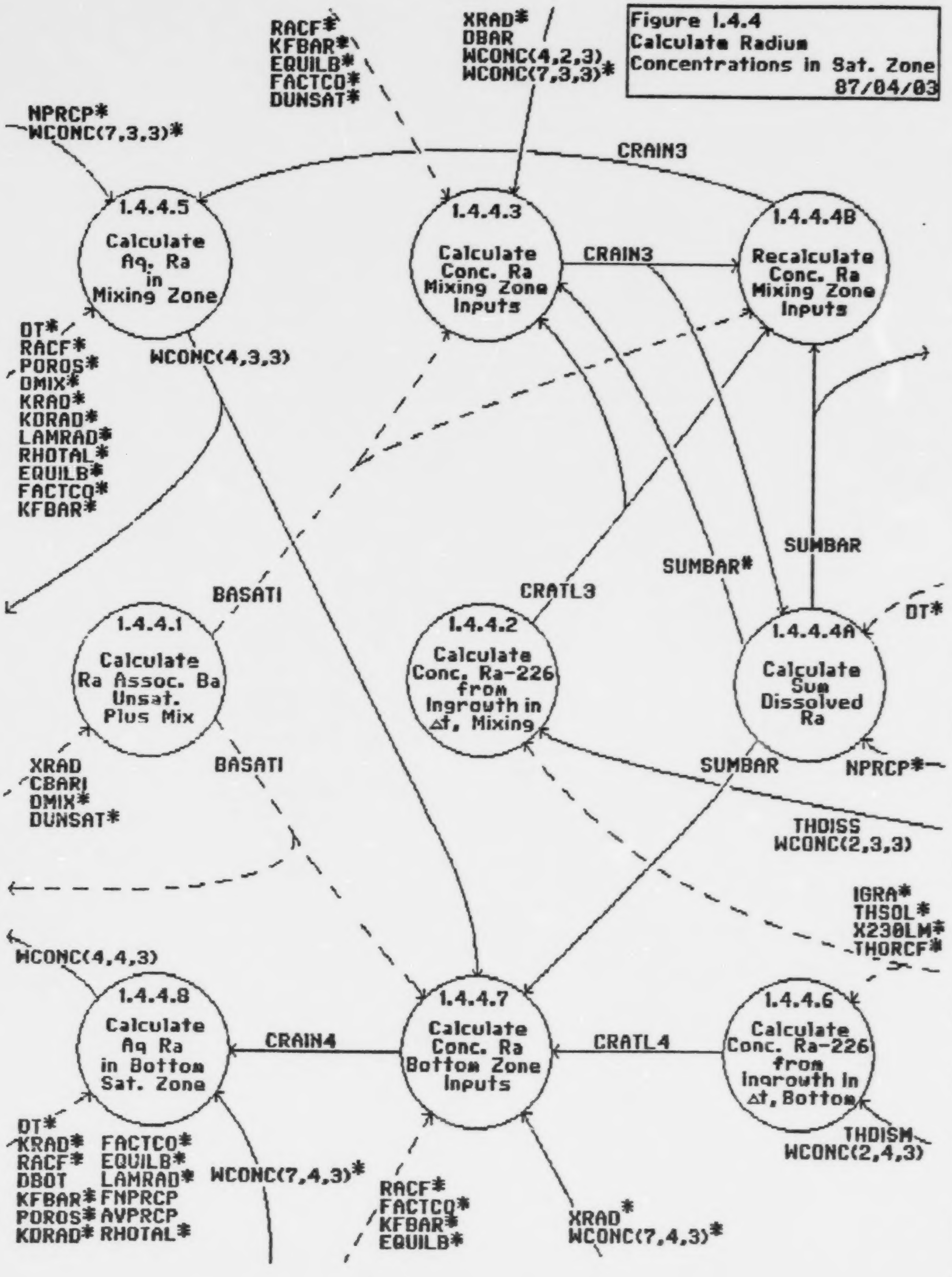


Figure 1.4.4
Calculate Radium
Concentrations in Sat. Zone
87/04/03

RACF*
KFBAR*
EQUILB*
FACTCO*
DUNSAT*
XRAD*
DBAR
WCONC(4,2,3)
WCONC(7,3,3)*
NPRCP*
WCONC(7,3,3)*
CRAIN3
1.4.4.5
Calculate Aq. Ra in Mixing Zone
1.4.4.3
Calculate Conc. Ra Mixing Zone Inputs
CRAIN3
1.4.4.4B
Recalculate Conc. Ra Mixing Zone Inputs
DT*
RACF*
POROS*
DMIX*
KRAD*
KDRAD*
LAMRAD*
RHOTAL*
EQUILB*
FACTCO*
KFBAR*
WCONC(4,3,3)
SUMBAR
SUMBAR*
CRATL3
BASATI
DT*
1.4.4.1
Calculate Ra Assoc. Ba Unsat. Plus Mix
1.4.4.2
Calculate Conc. Ra-226 from Ingrowth in Δt, Mixing
1.4.4.4A
Calculate Sum Dissolved Ra
XRAD
CBARI
DMIX*
DUNSAT*
BASATI
SUMBAR
NPRCP*
THDISS
WCONC(2,3,3)
IGRA*
THSOL*
X230LM*
THORCF*
WCONC(4,4,3)
1.4.4.8
Calculate Aq Ra in Bottom Sat. Zone
CRAIN4
1.4.4.7
Calculate Conc. Ra Bottom Zone Inputs
CRATL4
1.4.4.6
Calculate Conc. Ra-226 from Ingrowth in Δt, Bottom
THDISM
WCONC(2,4,3)
DT*
KRAD*
RACF*
DBOT
KFBAR*
POROS*
KDRAD*
FACTCO*
EQUILB*
LAMRAD*
FNPRCP
AVPRCP
RHOTAL*
WCONC(7,4,3)*
RACF*
FACTCO*
KFBAR*
EQUILB*
XRAD*
WCONC(7,4,3)*

Note: SUMBAR* is its value at the previous time step.

BASATI - INIT. RA ASSOC. BA UNSAT. PLUS MIX [mol m^{-2}]. The initial total radium associated with $BaSO_4$ in the unsaturated and mixing zones of the tailings.

Figure 1.4.4.1
Calculate INIT. RA ASSOC. BA UNSAT. PLUS MIX (BASATI)

XRADI
CBARI
DUNSAT - - -> BASATI
DMIX

Short Name	Long Name	SI Unit	Source
BASATI	INIT. RA ASSOC. BA UNSAT. PLUS MIX	[mol m^{-2}]	1.4.4.1
CBARI	INIT. SOLID CONC. $BASO_4$	[mol m^{-3}]	1.4.2.2
DMIX	THICKNESS OF MIXING ZONE	[m]	Sampled
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
XRADI	INIT. MOLE FRACT. RA-226	[-]	Sampled

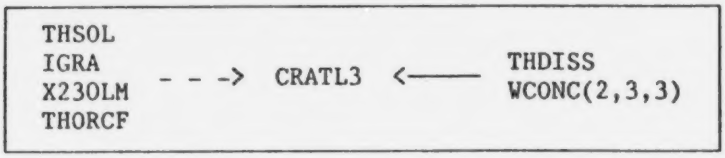
$$\text{BASATI} = \text{XRADI} * \text{CBARI} * (\text{DUNSAT} + \text{DMIX}) \qquad \text{(eqn. 3.7.39)}$$

Unit check:

$$\text{BASATI} \quad [-] * [\text{mol m}^{-3}] * ([\text{m}] + [\text{m}]) = [\text{mol m}^{-2}]$$

Figure 1.4.4.2
Calculate CONC. RA-226
FROM INGROWTH IN Δt,
MIXING (CRATL3)

CRATL3 - CONC. RA-226 FROM INGROWTH IN Δt, MIXING [mol m^{-3}]. The concentration of Ra-226 resulting from ingrowth from Th-230 in the mixing layer of the saturated zone during the time step Δt.



Short Name	Long Name	SI Unit	Source
CRATL3	CONC. RA-226 FROM INGROWTH IN Δt, MIXING	[mol m^{-3}]	1.4.4.2
IGRA	INGROWTH FACTOR FOR RA-226	[-]	1.4.1.1
THDISS	CONC. TOTAL TH DISS.	[mol m^{-3}]	1.3.2.1B
THORCF	WT. TH CONVERS. FACTOR	[Bq mol^{-1}]	1.3.1.11
THSOL	INIT. CONC. TOTAL SOLU. TH	[mol m^{-3}]	1.3.1.8
WCONC(2,3,3)	AQ. TH IN MIXING LAYER	[Bq m^{-3}]	1.3.2.7
X230LM	MOLE FRACT. TH-230	[-]	1.3.1.9

a) If $\text{THDISS} < \text{THSOL}$

$$\text{CRATL3} = 0$$

(eqn. 3.10.26; see Note 2)

b) If $\text{THDISS} \geq \text{THSOL}$ (see Note 2)

$$\text{CRATL3} = \text{X230LM} * \frac{\text{WCONC}(2,3,3) * \text{IGRA}}{\text{THORCF}}$$

(eqn. 3.10.27; (see Notes 1 & 2)

Unit check:

$$\text{CRATL3} \quad [-] * \frac{[\text{Bq m}^{-3}]}{[\text{Bq mol}^{-1}]} * [-] = [\text{mol m}^{-3}]$$

Note 1: The factor THORCF is required to convert WCONC(2,3,3) [Bq m^{-3}] to [mol m^{-3}]. The factor IGRA defined in Figure 1.4.1.1 has also been used to modify (simplify) equation (3.10.27).

Note 2: The summation sign in eqn. (3.10.26) is probably redundant. See equation (3.9.4).

Figure 1.4.4.3
Calculate CONC. RA MIXING ZONE INPUTS (CRAIN3)

CRAIN3 - CONC. RA MIXING ZONE INPUTS [mol m^{-3}]. The concentration of radium resulting from the various inputs to the mixing layer of the saturated zone.

RACF		WCONC(4,2,3)
EQUILB		XRAD
FACTCO		WCONC(7,3,3)
KFBAR	- - -> CRAIN3 <——	CRATL3
BASATI		SUMBAR(t-Δt)
DUNSAT		DBAR

Short Name	Long Name	SI Unit	Source
BASATI	INIT. RA ASSOC. BA UNSAT. PLUS MIX	[mol m^{-2}]	1.4.4.1
CRAIN3	CONC. RA MIXING ZONE INPUTS	[mol m^{-3}]	1.4.4.3
CRATL3	CONC. RA-226 FROM INGROWTH IN Δt, MIXING	[mol m^{-3}]	1.4.4.2
DBAR	THICKNESS $BASO_4$ DEPLETED LAYER	[m]	1.4.2.4
DUNSAT	DEPTH OF UNSAT. LAYER	[m]	Sampled
EQUILB	SQ. ROOT EQBM. CONST. $BASO_4$	[mol m^{-3}]	1.4.2.1
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
KFBAR	$BASO_4$ FORMATION CONSTANT	[m^3 mol^{-1}]	Sampled
RACF	CONVERSION FACTOR MOL TO BQ (RA-226)	[Bq mol^{-1}]	Sampled
SUMBAR	SUM DISSOLVED RA	[mol m^{-2}]	1.4.4.4
WCONC(4,2,3)	AQ. RA BOTTOM UNSAT. ZONE	[Bq m^{-3}]	1.4.3.5
WCONC(7,3,3)	CONC. OF SO_4 AQ. IN MIXING ZONE	[mol m^{-3}]	1.1.4.6
XRAD	MOLE FRACT. RA-226	[-]	1.4.3.1

(a) If SUMBAR(t-Δt) ≥ BASATI

$$\text{CRAIN3} = \text{CRATL3} \qquad \text{(eqn. 3.10.34)}$$

(b) If DBAR < DUNSAT and SUMBAR(t-Δt) < BASATI

$$\text{CRAIN3} = \frac{\text{WCONC}(4,2,3)}{\text{RACF}} + \text{CRATL3} \qquad \text{(eqn. 3.10.32)}$$

(c) If DBAR ≥ DUNSAT and SUMBAR(t-Δt) < BASATI

$$\text{CRAIN3} = \left(\frac{\text{EQUILB} * \text{EQUILB} * \text{XRAD}}{\text{EQUILB} + \text{WCONC}(7,3,3)}\right) * \left(1 + \text{KFBAR} * (\text{FACTCO})^2 * \text{WCONC}(7,3,3)\right) + \text{CRATL3}$$

(eqn. 3.10.33; see Note 2)

Unit check:

(a) $[\text{mol m}^{-3}] = [\text{mol m}^{-3}]$

(b) $$\frac{[\text{Bq m}^{-3}]}{[\text{Bq mol}^{-1}]} + [\text{mol m}^{-3}] = [\text{mol m}^{-3}]$$

(c) $$\frac{[\text{mol m}^{-3}] * [\text{mol m}^{-3}] * [-]}{[\text{mol m}^{-3}] + [\text{mol m}^{-3}]} * \left(1 + [\text{m}^3\ \text{mol}^{-1}] * [-]^2 * [\text{mol m}^{-3}]\right)$$

$$+ [\text{mol m}^{-3}] = [\text{mol m}^{-3}]$$

Note 1: The factor RACF is required to convert WCONC(4,2,3) from [Bq m^{-3}] to [mol m^{-3}].

Note 2: The calculation is also done for the time step from TIME=-Δt to TIME=0. Equation (3.7.43) is not used for layer 3 (SENES letter 1987-01-27).

SUMBAR - SUM DISSOLVED RA [mol m^{-2}].
Cumulative sum of radium inputs to the mixing zone to TIME=t.

Figure 1.4.4.4A
Calculate SUM
DISSOLVED RA
(SUMBAR)

$$\mathrm{DT}\equiv\Delta t \dashrightarrow \mathrm{SUMBAR}(t) \longleftarrow \begin{matrix}\mathrm{NPRCP}\\ \mathrm{CRAIN3}\\ \mathrm{SUMBAR}(t-\Delta t)\end{matrix}$$

Short Name	Long Name	SI Unit	Source
CRAIN3	CONC. RA MIXING ZONE INPUTS	[mol m^{-3}]	1.4.4.3
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled
SUMBAR	SUM DISSOLVED RA	[mol m^{-2}]	1.4.4.4A

From the finite difference equation

$$\mathrm{SUMBAR}(t) = \mathrm{SUMBAR}(t-\Delta t) + \mathrm{NPRCP} * \mathrm{CRAIN3} * \mathrm{DT} \quad \text{(eqn. 3.10.35)}$$

Unit check:

$$[\mathrm{mol\ m^{-2}}] + [\mathrm{m\ a^{-1}}] * [\mathrm{mol\ m^{-3}}] * [\mathrm{a}] = [\mathrm{mol\ m^{-2}}]$$

Note 1: Unit check failure. SENES reports [mol m^{-3}] for SUMBAR in Table A.3 but compares SUMBAR with BASATI [mol m^{-2}]. [mol m^{-2}] is correct (SENES letter 1986-12-02).

Note 2: SUMBAR = 0 at $t = -\Delta t$.

Figure 1.4.4.4B
Recalculate CONC. RA
MIXING ZONE INPUTS
(CRAIN3)

CRAIN3 - CONC. RA MIXING ZONE INPUTS [mol m^{-3}]. The concentration of radium resulting from the various inputs to the mixing layer of the saturated zone.

CRAIN3
BASATI - - -> CRAIN3 <—— SUMBAR(t)
CRATL3

Short Name	Long Name	SI Unit	Source
BASATI	INIT. RA ASSOC. BA UNSAT. PLUS MIX	[mol m^{-2}]	1.4.4.1
CRAIN3	CONC. RA MIXING ZONE INPUTS	[mol m^{-3}]	1.4.4.3, 1.4.4.4B
CRATL3	CONC. RA-226 FROM INGROWTH IN Δt, MIXING	[mol m^{-3}]	1.4.4.2
SUMBAR	SUM DISSOLVED RA	[mol m^{-2}]	1.4.4.4A

a) If SUMBAR(t) $\geq$ BASATI
CRAIN3 = CRATL3

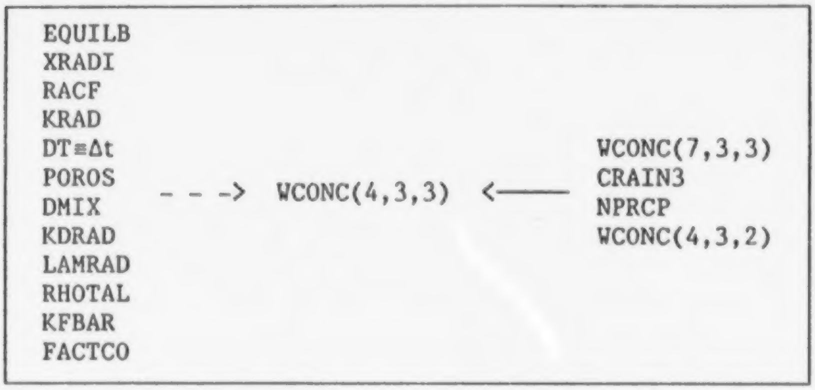
b) else CRAIN3 = CRAIN3 (eqn. 3.10.34)

Unit check:

$$[\text{mol } m^{-3}] = [\text{mol } m^{-3}]$$

WCONC(4,3,3) - AQ. RA IN MIXING LAYER [Bq m^{-3}]. The concentration of radium-226 in the aqueous phase in the mixing layer of the saturated zone.

Figure 1.4.4.5
Calculate AQ. RA IN
MIXING LAYER
(WCONC(4,3,3))
(Page 1 of 2)



Short Name	Long Name	SI Unit	Source
CRAIN3	CONC. RA MIXING ZONE INPUTS	[mol m^{-3}]	1.4.4.4B
DMIX	THICKNESS OF MIXING ZONE	[m]	Sampled
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
EQUILB	SQ. ROOT EQBM. CONST. $BASO_4$	[mol m^{-3}]	1.4.2.1
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
KDRAD	RA SOLID-LIQUID TRANSFER COEFFICIENT	[m^3 g^{-1}]	Sampled
KFBAR	$BASO_4$ FORMATION CONSTANT	[m^3 mol^{-1}]	Sampled
KRAD	RA SOLID/AQ. DIST. COEFFICIENT	[-]	Sampled
LAMRAD	RA-226 DECAY CONSTANT	[a^{-1}]	Sampled
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled
POROS	TAILINGS POROSITY	[-]	Sampled
RACF	CONVERSION FACTOR MOL TO BQ (RA-226)	[Bq mol^{-1}]	Sampled
RHOTAL	TAILINGS BULK DENSITY	[g m^{-3}]	Sampled
WCONC(4,3,2)	AQ. RA IN MIXING LAYER	[Bq m^{-3}]	(1.4.4.5)
WCONC(4,3,3)	AQ. RA IN MIXING LAYER	[Bq m^{-3}]	1.4.4.5
WCONC(7,3,3)	CONC. OF SO_4 AQ. IN MIXING LAYER	[mol m^{-3}]	1.1.4.4
XRADI	INIT. MOLE FRACT. RA-226	[-]	Sampled

If $t = 0$, WCONC(4,3,3) = XRADI * KRAD * CBARX1 * RACF where

$$\text{CBARX1} = \left(\frac{\text{EQUILB} * \text{EQUILB}}{\text{EQUILB} + \text{WCONC}(7,3,3)} * [1 + \text{FACTCO}^2 * \text{KFBAR} * \text{WCONC}(7,3,3)]\right)$$

(see Note 3)

Otherwise:

$$\text{WCONC}(4,3,3) = \text{RACF} * \left\{\text{CRAIN3} + \left[\frac{\text{WCONC}(4,3,2)}{\text{RACF}} * \text{EXP}(-\text{LAMRAD} * \text{DT}) - \text{CRAIN3}\right]\right.$$

$$\left. * \text{EXP}\left[\frac{-\text{NPRCP} * \text{DT}}{\text{POROS} * \text{DMIX}\left(1 + \frac{\text{KDRAD} * \text{RHOTAL}}{\text{POROS}}\right)}\right]\right\} \qquad \text{(eqn. 3.10.31)}$$

Unit check:

Initial condition: $[-] * [-] * [\text{mol m}^{-3}] * [\text{Bq mol}^{-1}] = [\text{Bq m}^{-3}]$

$$\text{CBARX1: } \frac{[\text{mol m}^{-3}] * [\text{mol m}^{-3}]}{[\text{mol m}^{-3}] + [\text{mol m}^{-3}]} * ([-] + [-]^2 * [\text{m}^3 \text{ mol}^{-1}] * [\text{mol m}^{-3}])$$

$$= [\text{mol m}^{-3}]$$

Figure 1.4.4.5
Calculate AQ. RA IN
MIXING LAYER
(WCONC(4,3,3))
(Page 2 of 2)

$$\mathrm{WCONC(4,4,3)}: \quad [\mathrm{Bq\ mol^{-1}}] * \Bigl\{ [\mathrm{mol\ m^{-3}}] + \Bigl[\frac{[\mathrm{Bq\ m^{-3}}]}{[\mathrm{Bq\ mol^{-1}}]} * \mathrm{EXP}([\mathrm{a^{-1}}] * [\mathrm{a}]) - [\mathrm{mol\ m^{-}}$$

$$* \ \mathrm{EXP} \left[\frac{-\ [\mathrm{m\ a^{-1}}] * [\mathrm{a}]}{[-] * [\mathrm{m}] * \left([-] + \frac{[\mathrm{m^3\ g^{-1}}]}{[-]} * [\mathrm{g\ m^{-3}}] \right)} \right] \Bigr] \Bigr\} = [\mathrm{Bq\ m^{-3}}]$$

Note 1: The factor RACF is required so that WCONC(4,3,3) is in units of [Bq m^{-3}].

Note 2: It is assumed WCONC(4,3,2) = 0 at t=0 but SENES clarification is required.

Note 3: The initial condition is taken from eqn. (3.7.44), and does not correspond to eqn. (3.10.31) at the limit t=0. The original specifications used only eqn. (3.10.31). (BWG, 87-04-09)

CRATL4 – CONC. RA-226 FROM INGROWTH IN Δt, BOTTOM [mol m^{-3}]. The concentration of Ra-226 resulting from ingrowth from Th-230 in the bottom layer of the saturated zone during the time step Δt.

Figure 1.4.4.6
Calculate CONC. RA-226
FROM INGROWTH IN Δt,
BOTTOM (CRATL4)

```
THSOL
IGRA                                 THDISM
X230LM  - - ->  CRATL4  <———         WCONC(2,4,3)
THORCF
```

Short Name	Long Name	SI Unit	Source
CRATL4	CONC. RA-226 FROM INGROWTH IN Δt, BOTTOM	[mol m^{-3}]	1.4.4.6
IGRA	INGROWTH FACTOR FOR RA-226	[-]	1.4.1.1
THDISM	CONC. TOTAL TH DISS. MIXING LAYER	[mol m^{-3}]	1.3.2.6B
THORCF	WT. TH CONVERS. FACTOR	[Bq mol^{-1}]	1.3.1.11
THSOL	INIT. CONC. TOTAL SOLU. TH	[mol m^{-3}]	1.3.1.8
WCONC(2,4,3)	AQ. TH IN BOTTOM SAT. ZONE	[Bq m^{-3}]	1.3.2.8
X230LM	MOLE FRACT. TH-230	[-]	1.3.1.9

a) If THDISM < THSOL

$$\text{CRATL4} = 0 \qquad \text{(eqn. 3.10.28)}$$

b) If THDISM $\geq$ THSOL

$$\text{CRATL4} = \text{X230LM} * \frac{\text{WCONC(2,4,3)}}{\text{THORCF}} * \text{IGRA} \qquad \text{(eqn. 3.10.29)}$$

Unit check:

b) $$[-] * \frac{[\text{Bq m}^{-3}]}{[\text{Bq mol}^{-1}]} * [-] = [\text{mol m}^{-3}]$$

Note 1: The factor THORCF is required to convert WCONC(2,4,3) [Bq m^{-3}] to [mol m^{-3}]. Furthermore, the factor IGRA defined in our figure 4.1.1.1 has been used to modify (simplify) equation (3.10.29).

Note 2: Clarification of equation (3.10.28) has been requested from SENES.

Figure 1.4.4.7
Calculate CONC. RA
BOTTOM ZONE INPUTS
(CRAIN4)

CRAIN4 - CONC. RA BOTTOM ZONE INPUTS [mol m^{-3}]. The concentration of radium resulting from the various inputs to the bottom layer of the saturated zone.

```
EQUILB                               WCONC(4,3,3)
RACF                                 XRAD
FACTCO  - - ->  CRAIN4  <------      CRATL4
KFBAR                                WCONC(7,4,3)
BASATI                               SUMBAR
```

Short Name	Long Name	SI Unit	Source
BASATI	INIT. RA ASSOC. BA UNSAT. PLUS MIX	[mol m^{-2}]	1.4.4.1
CRAIN4	CONC. RA BOTTOM ZONE INPUTS	[mol m^{-3}]	1.4.4.7
CRATL4	CONC. RA-226 FROM INGROWTH IN Δt, BOTTOM	[mol m^{-3}]	1.4.4.6
EQUILB	SQ. ROOT EQBM CONST. $BASO_4$	[mol m^{-3}]	1.4.2.1
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
KFBAR	$BASO_4$ FORMATION CONSTANT	[m^3 mol^{-1}]	Sampled
RACF	CONVERSION FACTOR MOL TO BQ (RA-226)	[Bq mol^{-1}]	Sampled
SUMBAR	SUM DISSOLVED RA	[mol m^{-2}]	1.4.4.4
WCONC(4,3,3)	AQ. RA IN MIXING LAYER	[Bq m^{-3}]	1.4.4.5
WCONC(7,4,3)	CONC. OF SO_4 AQ. IN BOTTOM LAYER	[mol m^{-3}]	1.1.5.3
XRAD	MOLE FRACT. RA-226	[-]	1.4.3.1

(a) If SUMBAR < BASATI

$$\text{CRAIN4} = \frac{\text{WCONC(4,3,3)}}{\text{RACF}} + \text{CRATL4} \qquad \text{(eqn. 3.10.38)}$$

(b) If SUMBAR ≥ BASATI

$$\text{CRAIN4} = \left(\frac{\text{EQUILB} * \text{EQUILB} * \text{XRAD}}{\text{EQUILB} + \text{WCONC(7,4,3)}}\right) * [1 + \text{KFBAR} * (\text{FACTCO})^2 * \text{WCONC(7,4,3)}] + \text{CRATL4}$$

(eqn. 3.10.39)

(see Note 2)

Unit check:

$$\text{(a)} \quad \frac{[\text{Bq m}^{-3}]}{[\text{Bq mol}^{-1}]} + [\text{mol m}^{-3}] = [\text{mol m}^{-3}]$$

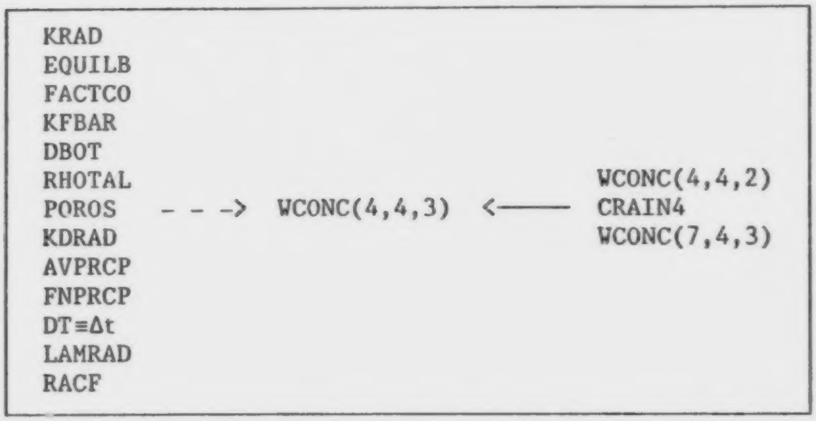
$$\text{(b)} \quad \left(\frac{[\text{mol m}^{-3}] * [\text{mol m}^{-3}] * [-]}{[\text{mol m}^{-3}] + [\text{mol m}^{-3}]}\right) * [-] + [\text{m}^3\ \text{mol}^{-1}] * [-]^2 * [\text{mol m}^{-3}]\Big) + [\text{mol m}^{-3}] = [\text{mol m}^{-3}]$$

Note 1: The factor RACF is required to convert WCONC(4,3,3) from [Bq m^{-3}] to [mol m^{-3}]. Furthermore equation (3.10.39) has been modified (simplified) by the use of the parameter EQUILB, defined as "a" below equation (3.10.6).

Note 2: The calculation is also done for the time step from TIME=-Δt to TIME=0. Equation (3.7.43) is not used for layer 3 (SENES letter 1987-01-27).

Figure 1.4.4.8
Calculate AQ. RA IN
BOTTOM SAT. ZONE
(WCONC(4,4,3))
(Page 1 of 2)

WCONC(4,4,3) - AQ. RA IN BOTTOM SAT. ZONE [Bq m^{-3}]. The concentration of Ra-226 in the aqueous phase at the bottom of the saturated zone.



Short Name	Long Name	SI Unit	Source
AVPRCP	AVERAGE NET PRECIPITATION	[m a^{-1}]	Sampled
CRAIN4	CONC. RA BOTTOM ZONE INPUTS	[mol m^{-3}]	1.4.4.7
DBOT	THICKNESS LAYER 4	[m]	1.1.1.4
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
EQUILB	SQ. ROOT EQBM. CONST. $BASO_4$	[mol m^{-3}]	1.4.2.1
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
FNPRCP	FRACT. NET PRECIP.	[-]	Sampled
KDRAD	RA SOLID-LIQUID TRANSFER COEFFICIENT	[m^3 g^{-1}]	Sampled
KFBAR	$BASO_4$ FORMATION CONSTANT	[m^3 mol^{-1}]	Sampled
KRAD	INIT. MOLE FRACT. RA-226	[-]	Sampled
LAMRAD	RA-226 DECAY CONSTANT	[a^{-1}]	Sampled
POROS	TAILINGS POROSITY	[-]	Sampled
RACF	CONVERSION FACTOR MOL TO BQ (RA-226)	[Bq mol^{-1}]	Sampled
RHOTAL	TAILINGS BULK DENSITY	[g m^{-3}]	Sampled
WCONC(4,4,2)	AQ. RA IN BOTTOM SAT. ZONE	[Bq m^{-3}]	1.4.4.8
WCONC(4,4,3)	AQ. RA IN BOTTOM SAT. ZONE	[Bq m^{-3}]	1.4.4.8
WCONC(7,4,3)	CONC. OF SO_4 AQ. IN BOTTOM LAYER	[mol m^{-3}]	1.1.5.3

If $t=0$, WCONC(4,4,3) = XRADI * CBARX2 * KRAD * RACF

$$\text{where CBARX2} = \frac{\text{EQUILB}^2}{\text{EQUILB} + \text{WCONC}(7,4,3)} * (1 + \text{FACTCO}^2 * \text{KFBAR} * \text{WCONC}(7,4,3))$$

(see Note 4)

$$\text{Otherwise WCONC}(4,4,3) = \text{RACF} * \left\{\text{CRAIN4} + \left[\frac{\text{WCONC}(4,4,2)}{\text{RACF}} * \text{EXP}(-\text{LAMRAD} * \text{DT}) - \text{CRAIN4}\right] * \text{EXP}\left[\frac{-\text{FNPRCP} * \text{AVPRCP} * \text{DT}}{\text{POROS} * \text{DBOT} * \left(1 + \frac{\text{KDRAD} * \text{RHOTAL}}{\text{POROS}}\right)}\right]\right\} \quad \text{(eqn. 3.10.37)}$$

Figure 1.4.4.8
Calculate AQ. RA IN
BOTTOM SAT. ZONE
(WCONC(4,4,3))
(Page 2 of 2)

Unit check:

$$\text{Initial condition:}\quad [-] * [\text{mol m}^{-3}] * [-] * [\text{Bq mol}^{-1}] = [\text{Bq m}^{-3}]$$

$$\begin{aligned}\text{CBARX2:}\quad & \frac{[\text{mol m}^{-3}]^2}{[\text{mol m}^{-3}] + [\text{mol m}^{-3}]} * ([-] + [-]^2 + [\text{m}^3\ \text{mol}] * [\text{mol m}^{-3}] \\ & = [\text{mol m}^{-3}]\end{aligned}$$

$$\begin{aligned}\text{WCONC(4,4,3):}\quad & [\text{Bq mol}^{-1}] * \Bigg\{[\text{mol m}^{-3}] + \left[\frac{[\text{Bq m}^{-3}]}{[\text{Bq mol}^{-1}]} * \exp\,([\text{a}^{-1}] * [\text{a}])\right. \\ & \left. - [\text{mol m}^{-3}]\right] * \text{EXP}\left[\frac{-[-] * [\text{m a}^{-1}] * [\text{a}]}{[-] * [\text{m}] * \left([-] + \frac{[\text{m}^3\ \text{g}^{-1}] * [\text{g m}^{-3}]}{[-]}\right)}\right]\Bigg\} = [\text{Bq m}^{-3}]\end{aligned}$$

Note 1: The factor RACF is required so that WCONC(4,4,3) is in units of [Bq m^{-3}].

Note 2: "f" used in equation (3-90) is assumed to be FNPRCP (f_p) from the definition on page (3-90), not FACTCO which is defined as "f" in Table A.3.

Note 3: Clarification on the initial condition has been requested from SENES but WCONC(4,4,2) = 0 at t=0 has been assumed.

Note 4: The initial condition is taken from eqn. (3.7.44), and does not correspond to eqn. (3.10.31) at the limit t=0. The original specification used only eqn. (3.10.31). (BWG, 87-04-09)

Note 5: See also response #81 in Appendix A.

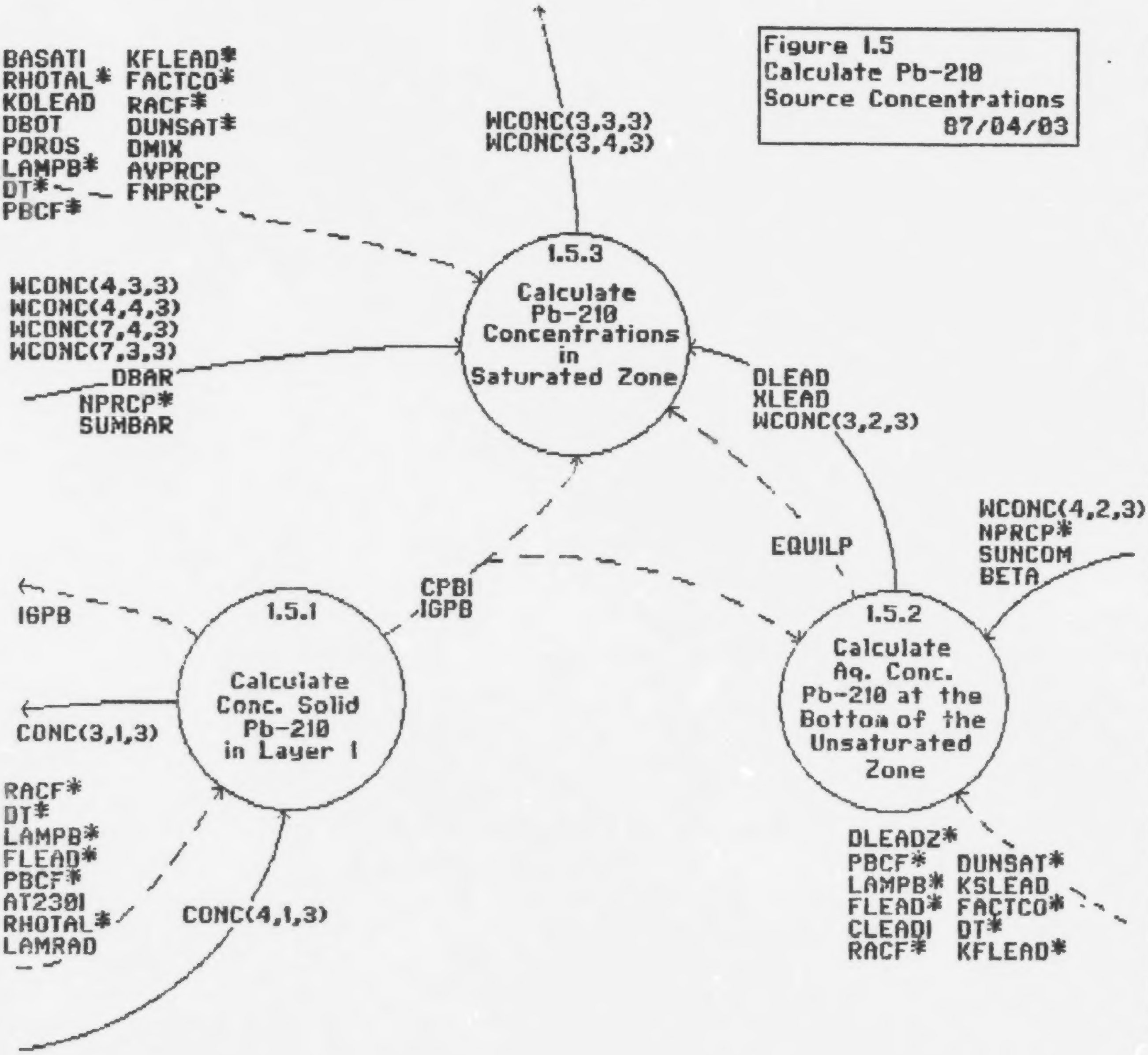


Figure 1.5
Calculate Pb-210
Source Concentrations
87/04/03

BASATI
RHOTAL*
KDLEAD
DBOT
POROS
LAMPB*
DT*
PBCF*
KFLEAD*
FACTCO*
RACF*
DUNSAT*
DMIX
AVPRCP
FNPRCP
WCONC(3,3,3)
WCONC(3,4,3)
1.5.3
Calculate
Pb-210
Concentrations
in
Saturated Zone
WCONC(4,3,3)
WCONC(4,4,3)
WCONC(7,4,3)
WCONC(7,3,3)
DBAR
NPRCP*
SUMBAR
DLEAD
XLEAD
WCONC(3,2,3)
WCONC(4,2,3)
NPRCP*
SUNCOM
BETA
EQUILP
CPBI
IGPB
IGPB
1.5.1
Calculate
Conc. Solid
Pb-210
in Layer 1
CONC(3,1,3)
RACF*
DT*
LAMPB*
FLEAD*
PBCF*
AT230I
RHOTAL*
LAMRAD
CONC(4,1,3)
1.5.2
Calculate
Aq. Conc.
Pb-210 at the
Bottom of the
Unsaturated
Zone
DLEADZ*
PBCF*
LAMPB*
FLEAD*
CLEADI
RACF*
DUNSAT*
KSLEAD
FACTCO*
DT*
KFLEAD*

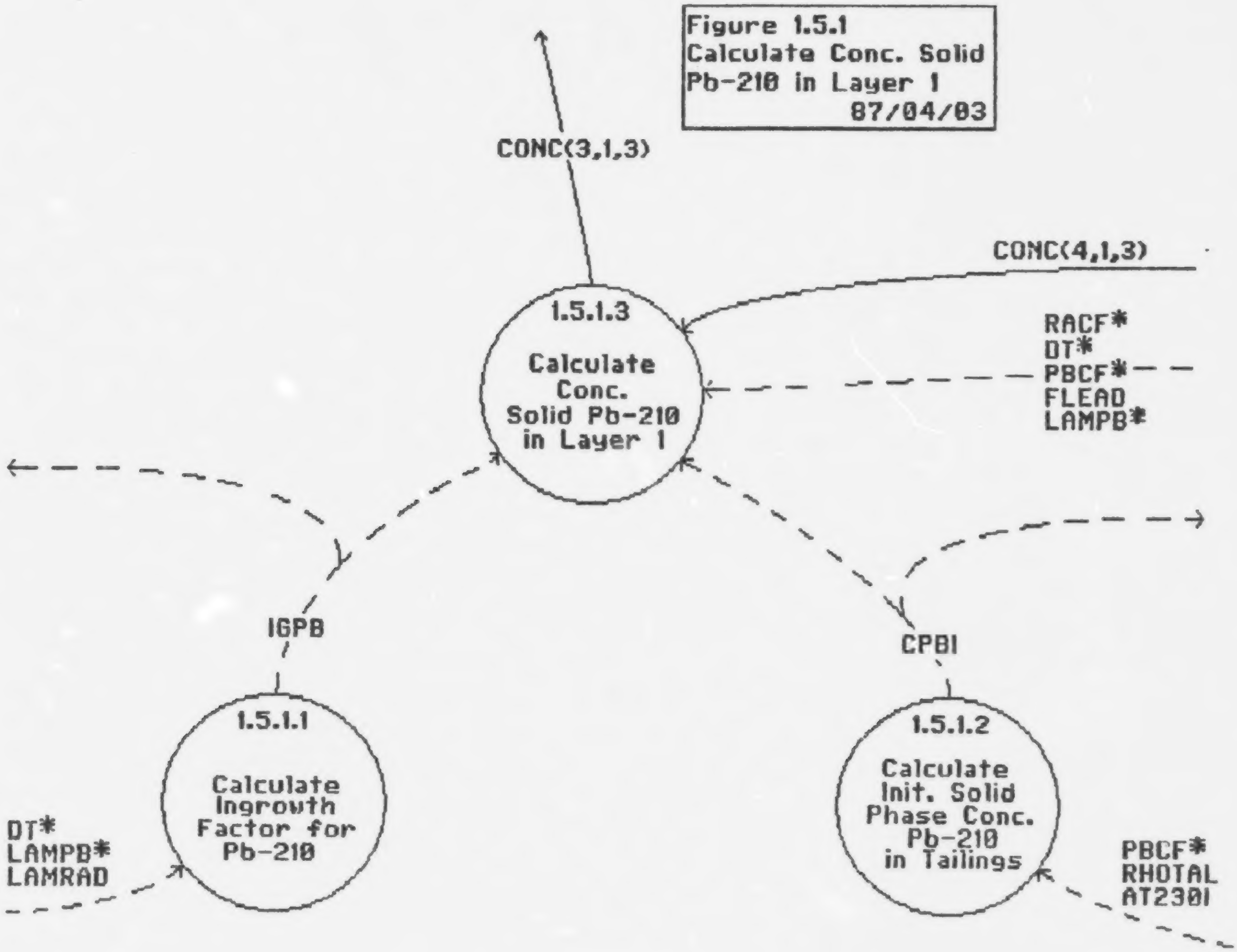


Figure 1.5.1
Calculate Conc. Solid
Pb-210 in Layer 1
87/04/03

CONC(3,1,3)
CONC(4,1,3)
1.5.1.3
Calculate
Conc.
Solid Pb-210
in Layer 1
RACF*
DT*
PBCF*
FLEAD
LAMPB*
IGPB
CPBI
1.5.1.1
Calculate
Ingrowth
Factor for
Pb-210
DT*
LAMPB*
LAMRAD
1.5.1.2
Calculate
Init. Solid
Phase Conc.
Pb-210
in Tailings
PBCF*
RHOTAL
AT230I

IGPB - INGROWTH FACTOR FOR PB-210 [-].
The factor used to approximate the ingrowth of Pb-210 from Ra-226.

Figure 1.5.1.1
Calculate INGROWTH
FACTOR FOR PB-210
(IGPB)

LAMRAD
LAMPB - - - > IGPB
DT≡Δt

Short Name	Long Name	SI Unit	Source
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
IGPB	INGROWTH FACTOR FOR PB-210	[-]	1.5.1.1
LAMPB	PB-210 DECAY CONSTANT	$[a^{-1}]$	Sampled
LAMRAD	RA-226 DECAY CONSTANT	$[a^{-1}]$	Sampled

$$\text{IGPB} = \left(\frac{\text{LAMRAD}}{\text{LAMPB-LAMRAD}}\right) * \left[\text{EXP(-LAMRAD*DT)-EXP(-LAMPB*DT)}\right]$$

(Part of eqn. 3.11.10)

Unit check:

$$\left(\frac{[a^{-1}]}{[a^{-1}]-[a^{-1}]}\right) * \left[\text{EXP}([a^{-1}] * [a])-\text{EXP}([a^{-1}] * [a])\right] = [-]$$

Note: This factor is not defined by SENES but was defined here for convenience. It is used in several equations in the TSOURC modules and elsewhere.

Figure 1.5.1.2
Calculate INIT. SOLID
PHASE CONC. PB-210 IN
TAILINGS (CPBI)

CPBI - INIT. SOLID PHASE CONC. PB-210 IN TAILINGS [mol m^{-3}]. The initial solid phase concentration of Pb-210 in the tailings.

```
APBI
PBCF     - - - >   CPBI
RHOTAL

AT230I   - - - >   APBI
```

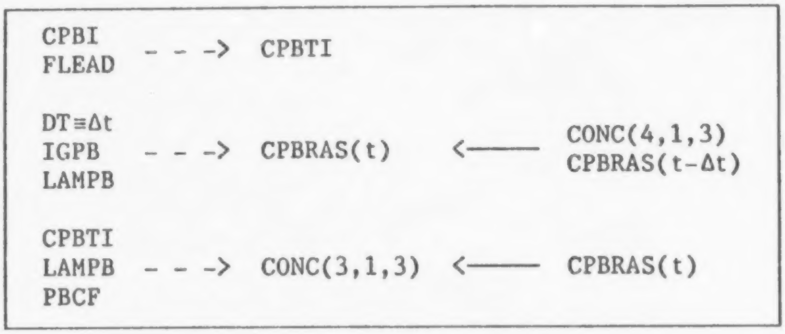
Short Name	Long Name	SI Unit	Source
APBI	INIT. ACTIV. PB-210 IN TAILINGS	[Bq g^{-1}]	(1.5.1.2)
AT230I	INIT. ACTIV. TH-230 IN TAILINGS	[Bq g^{-1}]	1.3.1.1
CPBI	INIT. SOLID PHASE CONC. PB-210 IN TAILINGS	[mol m^{-3}]	1.5.1.2
PBCF	CONVERSION FACTOR MOL TO BQ (PB-210)	[Bq mol^{-1}]	Sampled
RHOTAL	TAILINGS BULK DENSITY	[g m^{-3}]	Sampled

CPBI = APBI*RHOTAL/PBCF (eqn. 3.7.47)
APBI = AT230I (eqn. 3.7.45, 3.7.33)

Unit checks:
CPBI: [Bq g^{-1}] * [g m^{-3}]/[Bq mol^{-1}] = [mol m^{-3}]
APBI: [Bq g^{-1}] = [Bq g^{-1}]

CONC(3,1,3) - CONC. SOLID PB-210 IN LAYER 1 [Bq m^{-3}]. Solid phase concentration of lead-210 in the upper layer of the unsaturated zone.

Figure 1.5.1.3
Calculate CONC. SOLID
PB-210 IN LAYER 1
(CONC(3,1,3))



Short Name	Long Name	SI Unit	Source
CONC(3,1,3)	CONC. SOLID PB-210 IN LAYER 1	[Bq m^{-3}]	1.5.1.3
CONC(4,1,3)	CONC. SOLID RA IN LAYER 1	[Bq m^{-3}]	1.4.1.4
CPBI	INIT. SOLID PHASE CONC. PB-210 IN TAILINGS	[mol m^{-3}]	1.5.1.2
CPBTI	INIT. CONC. PB-210 ASSOC. WITH HOST TAILINGS	[mol m^{-3}]	(1.5.1.3)
CPBRAS	CUM. SOLID CONC. PB-210 FROM RA-226	[mol m^{-3}]	(1.5.1.3)
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
FLEAD	FRACT. PB SOLUBLE	[-]	Sampled
IGPB	INGROWTH FACTOR FOR PB-210	[-]	1.5.1.1
LAMPB	PB-210 DECAY CONSTANT	[a^{-1}]	Sampled
PBCF	CONVERSION FACTOR MOL TO BQ (PB-210)	[Bq mol^{-1}]	Sampled

If t>0 CONC(3,1,3) = (CPBTI * EXP(-LAMPB * TIME) + CPBRAS(t)) * PBCF (eqn. 3.11.8)

If t=0 CONC(3,1,3) = CPBTI * PBCF (eqn. 3.7.51)

Solve the following finite difference equation for CPBRAS:

$$\text{CPBRAS}(t) = \text{CPBRAS}(t-\Delta t) * \text{EXP}(-\text{LAMPB*DT}) + \frac{\text{CONC}(4,1,3)}{\text{RACF}}\text{*IGPB} \qquad \text{(eqn. 3.11.7; see Note 1)}$$

$$\text{CPBTI} = (1.-\text{FLEAD})\text{*CPBI} \qquad \text{(eqn. 3.7.49)}$$

Unit checks:

CONC(3,1,3): ([mol m^{-3}] * EXP([a^{-1}] * [a]) + [mol m^{-3}]) * [Bq mol^{-1}] = [Bq m^{-3}]

CPBRAS : [mol m^{-3}] * EXP([a^{-1}] * [a]) + $\frac{[\text{Bq m}^{-3}]}{[\text{Bq mol}^{-1}]}$ * [-] = [mol m^{-3}]

CPBTI : ([-] - [-]) * [mol m^{-3}] = [mol m^{-3}]

Note 1: Equation (3.11.7) in the SENES report is missing parentheses around the last two exponential factors (incorporated here into the term IGPB).
(SENES letter 1986-12-02)

Note 2: The factor PBCF is required in the equations for CPBRAS and CONC(3,1,3) to maintain consistency of units.

Note 3: It is assumed $[\text{Ra-226}_s]_1 \equiv [\text{Ra}_s]_1 \equiv$ CONC(4,1,3).

Note 4: Assume that CPBRAS(t=0) is zero (BWG, 87-03-17). This assumption agrees with the UTAP2 code (BWG, 87-04-02).

Note 5: Inspection of the UTAP2 code shows that a logic error has:
CONC(3,1,3) = CPBRAS * PBCF
for t>0. This error is reproduced in SYVAC3-UT2. (BWG, 87-03-07).

Figure 1.5.2
Calculate Aq. Conc. Pb-210
at the Bottom of the
Unsaturated Zone
87/04/06

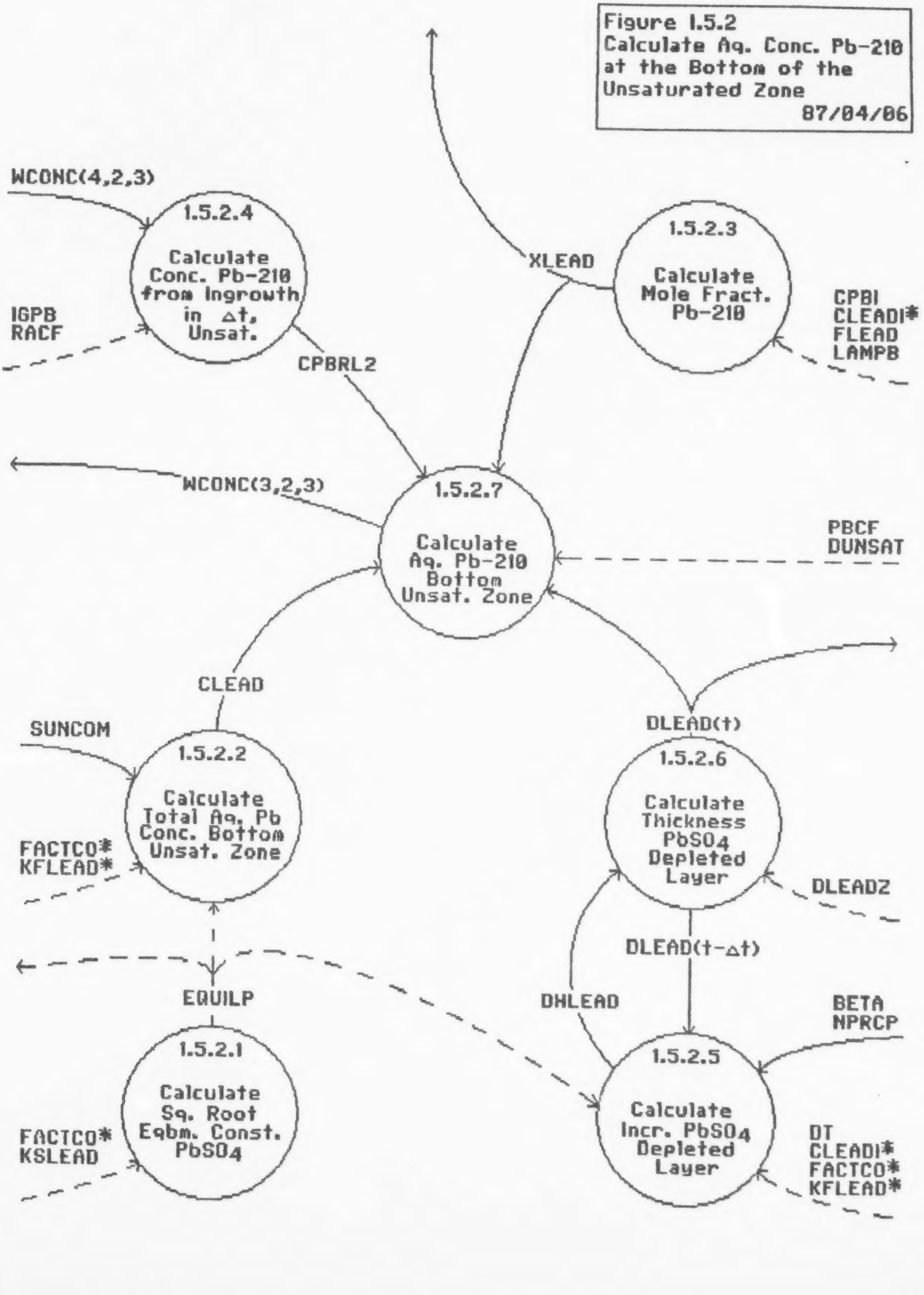

WCONC(4,2,3)
1.5.2.4
Calculate Conc. Pb-210 from Ingrowth in ∆t, Unsat.
IGPB
RACF
CPBRL2
XLEAD
1.5.2.3
Calculate Mole Fract. Pb-210
CPBI
CLEADI*
FLEAD
LAMPB
WCONC(3,2,3)
1.5.2.7
Calculate Aq. Pb-210 Bottom Unsat. Zone
PBCF
DUNSAT
CLEAD
DLEAD(t)
SUNCOM
1.5.2.2
Calculate Total Aq. Pb Conc. Bottom Unsat. Zone
FACTCO*
KFLEAD*
1.5.2.6
Calculate Thickness PbSO4 Depleted Layer
DLEADZ
DLEAD(t-∆t)
EQUILP
DHLEAD
BETA
NPRCP
1.5.2.1
Calculate Sq. Root Eqbm. Const. PbSO4
FACTCO*
KSLEAD
1.5.2.5
Calculate Incr. PbSO4 Depleted Layer
DT
CLEADI*
FACTCO*
KFLEAD*

Figure 1.5.2.1
Calculate
SQ. ROOT EQBM. CONST.
(EQUILP)

EQUILP - SQ. ROOT EQBM. CONST. PBSO4 [mol m^{-3}]. EQUILP is an intermediate variable, equal to the square root of the solubility product for lead sulphate, divided by the activity coefficient.

FACTCO
KSLEAD - - - > EQUILP

Short Name	Long Name	SI Unit	Source
EQUILP	SQ. ROOT OF EQBM. CONST. PBSO4	[mol m^{-3}]	1.5.2.1
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
KSLEAD	SOLUBILITY EQM. CONST. FOR PBSO4	[mol^2 m^{-6}]	Sampled

$$\mathrm{EQUILP} = \sqrt{\frac{\mathrm{KSLEAD}}{(\mathrm{FACTCO})^2}} \qquad \text{(eqn. near 3.11.4)}$$

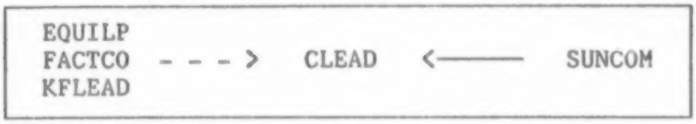
Unit check

$$\left(\frac{[\mathrm{mol}^2 \mathrm{m}^{-6}]}{[-]}\right)^{0.5} = [\mathrm{mol\ m}^{-3}]$$

Note 1: EQUILP is equivalent to symbol "a" in the text, but is not defined in Table A.3. "a" is defined as EQUIL in Table A.3 and with three different meanings in different places in the text.

Figure 1.5.2.2
Calculate TOTAL AQ. PB
CONC. BOTTOM UNSAT.
ZONE (CLEAD)

CLEAD - TOTAL AQ. PB CONC. BOTTOM UNSAT. ZONE [mol m-3]. Total concentration of dissolved lead at the bottom of the unsaturated zone.



Short Name	Long Name	SI Unit	Source
CLEAD	TOTAL AQ. PB CONC. BOTTOM UNSAT. ZONE	$[mol\ m^{-3}]$	1.5.2.2
EQUILP	SQ. ROOT EQBM. CONST. PBSO4	$[mol\ m^{-3}]$	1.5.2.1
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
KFLEAD	PBSO4(AQ) FORMATION CONSTANT	$[m^3\ mol^{-1}]$	Sampled
SUNCOM	CONC. UNCOMP. SO4 BOTTOM UNSAT. ZONE	$[mol\ dm^{-3}]$	1.1.2.12

$$CLEAD = \left(\frac{EQUILP*EQUILP}{EQUILP + SUNCOM*1000}\right) * (1+(FACTCO)^2*KFLEAD*SUNCOM*1000)$$

(eqn. 3.11.1)

Unit check:

$$\frac{[mol\ m^{-3}]^2}{[mol\ m^{-3}] + [mol\ dm^{-3}] * [dm^3\ m^{-3}]} (1+[-]^2[m^3\ mol^{-1}][mol\ dm^{-3}][dm^3\ m^{-3}])$$

$$= [mol\ m^{-3}]$$

Note 1: The factors of 1000 $[dm^3\ m^{-3}]$ are required to express the concentrations of uncomplexed sulphate in $[mol\ m^{-3}]$.

Note 2: Equation (3.11.1) has been modified here by the use of EQUILP, defined near equation (3.11.4).

Figure 1.5.2.3
Calculate
MOLE FRACT. PB-210
(XLEAD)

XLEAD - MOLE FRACT. PB-210 [-]. Mole fraction of $^{210}PbSO_4$ in the lead sulphate, corrected for decay of Pb-210.

XPBI
LAMPB ---> XLEAD

FLEAD
CLEADI ---> XPBI
CPBI

Short Name	Long Name	SI Unit	Source
CLEADI	INITIAL CONC. PB	[mol m^{-3}]	Sampled
CPBI	INIT. SOLID PHASE CONC. PB-210 IN TAILINGS	[mol m-3]	1.5.1.2
FLEAD	FRACT. PB SOLUBLE	[-]	Sampled
LAMPB	PB-210 DECAY CONSTANT	[a^{-1}]	Sampled
XLEAD	MOLE FRACT. PB-210	[-]	1.5.2.3
XPBI	INIT. MOLE FRACT. PB-210	[-]	(1.5.2.3)

$$\text{XLEAD} = \text{XPBI*EXP(-LAMPB*TIME)} \qquad \text{(eqn. below 3.11.2)}$$

$$\text{XPBI} = \frac{\text{FLEAD*CPBI}}{\text{CLEADI}} \qquad \text{(eqns. 3.7.48 and 3.7.50)}$$

Unit check:

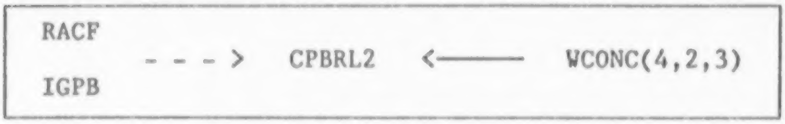
$$\text{XLEAD:} \quad [-] * \text{EXP}([a^{-1}] * [a]) = [-]$$

$$\text{XPBI:} \quad [-] * \frac{[\text{mol m}^{-3}]}{[\text{mol m}^{-3}]} = [-]$$

Note 1: Inspection of the UTAP2 code shows that a logic error has XLEAD=0 for t>0. This error is reproduced in SYVAC3-UT2. (BWG, 87-03-07) It is also assumed that XLEAD=0 at t=0. (BWG)

Figure 1.5.2.4
Calculate CONC. PB-210 FROM INGROWTH IN ΔT, UNSAT. (CPBRL2)

CPBRL2 - CONC. PB-210 FROM INGROWTH IN ΔT, UNSAT. [mol m^{-3}]. The concentration of Pb-210 at the bottom of the unsaturated zone resulting from ingrowth from dissolved Ra-226 during the time step Δt.



Short Name	Long Name	SI Unit	Source
CPBRL2	CONC. PB-210 FROM INGROWTH IN ΔT, UNSAT.	[mol m^{-3}]	1.5.2.4
IGPB	INGROWTH FACTOR FOR PB-210	[-]	1.5.1.1
RACF	CONVERSION FACTOR MOL TO BQ (RA-226)	[Bq mol^{-1}]	Sampled
WCONC(4,2,3)	AQ. RA BOTTOM UNSAT. ZONE	[Bq m^{-3}]	1.4.3.5

$$\mathrm{CPBRL2} = \frac{\mathrm{WCONC(4,2,3)}}{\mathrm{RACF}} * \mathrm{IGPB} \qquad \text{(eqn. 3.11.3)}$$

Unit check

$$\mathrm{CPBRL2} \qquad \frac{[\mathrm{Bq\ m^{-3}}]}{[\mathrm{Bq\ mol^{-1}}]} * [-] = [\mathrm{mol\ m^{-3}}]$$

Note: The factor RACF is required to convert the radium concentration WCONC(4,2,3) from [Bq m^{-3}] to [mol m^{-3}].

DHLEAD - INCR. PBSO4 DEPLETED LAYER [m].
Increase in the thickness of the lead sulphate depleted layer over the time interval Δt.

Figure 1.5.2.5
Calculate INCR. PBSO4
DEPLETED LAYER
(DHLEAD)

$$\begin{array}{lcccl} \text{FACTCO} & & & & \\ \text{EQUILP} & & & & \text{BETA} \\ \text{DT}\equiv\Delta t & \dashrightarrow & \text{DHLEAD(t)} & \longleftarrow & \text{NPRCP} \\ \text{CLEADI} & & & & \text{DLEAD}(t-\Delta t) \\ \text{KFLEAD} & & & & \end{array}$$

Short Name	Long Name	SI Unit	Source
BETA	PYRITE OXIDATION FACTOR	$[\text{mol m}^{-3}]$	1.1.2.4
CLEADI	INITIAL CONC. PB	$[\text{mol m}^{-3}]$	Sampled
DHLEAD	INCR. PBSO4 DEPLETED LAYER	[m]	1.5.2.5
DLEAD	THICKNESS PBSO4 DEPLETED LAYER	[m]	1.5.2.6
DT≡ΔT	TIME STEP-SIZE	[a]	Sampled
EQUILP	SQ. ROOT EQBM. CONST. PBSO4	$[\text{mol m}^{-3}]$	1.5.2.1
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
KFLEAD	PBSO4(AQ) FORMATION CONSTANT	$[\text{m}^3\ \text{mol}^{-1}]$	Sampled
NPRCP	NET PRECIPITATION	$[\text{m a}^{-1}]$	Sampled

For t>0

$$\begin{aligned} \text{DHLEAD}(t) = {} & \left\{ \frac{(\text{EQUILP})^2 * \text{NPRCP} * \text{DT}}{\text{CLEADI}} * \left[\frac{\text{NPRCP} * \text{DT}}{\text{BETA}} + 2 * (\text{FACTCO})^2 * \text{KFLEAD} * \text{DLEAD}(t-\Delta t) \right] \right. \\ & \left. + \frac{1}{4} \left[2 * \text{DLEAD}(t-\Delta t) + \frac{\text{EQUILP} * \text{NPRCP} * \text{DT}}{\text{BETA}} - \frac{(\text{EQUILP})^2 * (\text{FACTCO})^2 * (\text{KFLEAD}) * \text{NPRCP} * \text{DT}}{\text{CLEADI}} \right]^2 \right\}^{0.5} \\ & - \left[\text{DLEAD}(t-\Delta t) + \frac{\text{EQUILP} * \text{NPRCP} * \text{DT}}{2 * \text{BETA}} - \frac{(\text{EQUILP})^2 * (\text{FACTCO})^2 * (\text{KFLEAD}) * \text{NPRCP} * \text{DT}}{2 * \text{CLEADI}} \right] \end{aligned}$$

(eqn. 3.11.4)

Unit check

$$\begin{aligned} \text{DHLEAD} & \left\{ \frac{[\text{mol m}^{-3}]^2 * [\text{m a}^{-1}][\text{a}]}{[\text{mol m}^{-3}]} * \left[\frac{[\text{m a}^{-1}] * [\text{a}]}{[\text{mol m}^{-3}]} + [-]^2 * [\text{m}^3\ \text{mol}^{-1}] * [\text{m}] \right] \right. \\ & \left. + \left[[\text{m}] + \frac{[\text{mol m}^{-3}] * [\text{m a}^{-1}] * [\text{a}]}{[\text{mol m}^{-3}]} - \frac{[\text{mol m}^{-3}]^2 * [-]^2 * [\text{m}^3\ \text{mol}^{-1}] * [\text{m a}^{-1}] * [\text{a}]}{[\text{mol m}^{-3}]} \right]^2 \right\}^{0.5} \\ & - \left[[\text{m}] + \frac{[\text{mol m}^{-3}] * [\text{m a}^{-1}] * [\text{a}]}{[\text{mol m}^{-3}]} - \frac{[\text{mol m}^{-3}]^2 * [-]^2 * [\text{m}^3\ \text{mol}^{-1}] * [\text{m a}^{-1}] * [\text{a}]}{[\text{mol m}^{-3}]} \right] = [\text{m}] \end{aligned}$$

Note: DHLEAD and DLEAD are not calculated at TIME=(-Δt) or TIME=0.
DLEAD(t=0) is 0.01 [m] (SENES Vol. 3 pg. 3-93).

DLEAD - THICKNESS PBSO4 DEPLETED LAYER [m].
The thickness of the lead sulphate depleted layer of the tailings.

Figure 1.5.2.6
Calculate THICKNESS PBSO4 DEPLETED LAYER (DLEAD)

$$\text{DLEADZ} \dashrightarrow \text{DLEAD}(t) \longleftarrow \begin{array}{l}\text{DLEAD}(t-\Delta t)\\ \text{DHLEAD}\end{array}$$

Short Name	Long Name	SI Unit	Source
DHLEAD	INCR. PBSO4 DEPLETED LAYER	[m]	1.5.2.5
DLEAD	THICKNESS PBSO4 DEPLETED LAYER	[m]	1.5.2.6
DLEADZ	THICKNESS PBSO4 DEPLETED LAYER AT TIME=0	[m]	Sampled

if TIME = 0.0
DLEAD = DLEADZ (SENES pg 3-93)

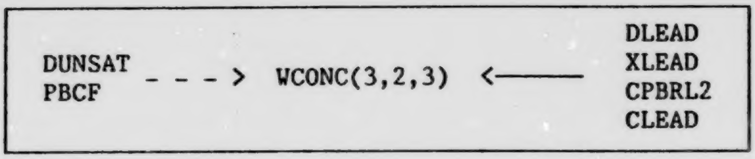
if TIME > 0.0 from the finite difference equation:
DLEAD (TIME=t) = DLEAD (TIME=(t-Δt)) + DHLEAD (eqn. 3.11.5)

Unit check:

$$[m] + [m] = [m]$$

Figure 1.5.2.7
Calculate AQ. PB-210
BOTTOM UNSAT. ZONE
(WCONC(3,2,3))

WCONC(3,2,3) - AQ. PB-210 BOTTOM UNSAT. ZONE [Bq m^{-3}]. The concentration of lead-210 in the aqueous phase at the bottom of the unsaturated zone.



Short Name	Long Name	SI Unit	Source
CLEAD	TOTAL AQ. PB CONC. BOTTOM UNSAT. ZONE	[mol m^{-3}]	1.5.2.2
CPBRL2	CONC. PB-210 FROM INGROWTH IN ΔT, UNSAT.	[mol m^{-3}]	1.5.2.4
DLEAD	THICKNESS OF PBSO4 DEPLETED LAYER	[m]	1.5.2.6
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
PBCF	CONVERSION FACTOR MOL TO BQ (PB-210)	[Bq mol^{-1}]	Sampled
WCONC(3,2,3)	AQ. PB-210 BOTTOM UNSAT. ZONE	[Bq m^{-3}]	1.5.2.7
XLEAD	MOL FRACT. PB-210	[-]	1.5.2.3

If t=0 then WCONC(3,2,3) = XLEAD * CLEAD * PBCF (see Note 2)

otherwise:

if DLEAD < DUNSAT
WCONC(3,2,3) = (XLEAD * CLEAD + CPBRL2) * PBCF (eqn. 3.11.2)

if DLEAD $\geq$ DUNSAT
WCONC(3,2,3) = CPBRL2 * PBCF (eqn. 3.11.6)

Unit check:
$$([-] * [\text{mol m}^{-3}] + [\text{mol m}^{-3}]) * [\text{Bq mol}^{-1}] = [\text{Bq m}^{-3}]$$

Note 1: The factor PBCF [Bq mol^{-1}] has been used to maintain the units of WCONC(3,2,3) as [Bq m^{-3}].

Note 2: Initial condition deduced from an inspection of the UTAP2 code. It is also given in eqn. (3.7.51) (BWG, 87-04-02).

Figure 1.5.3
Calculate Pb-210
Concentrations in
Saturated Zone
87/04/07

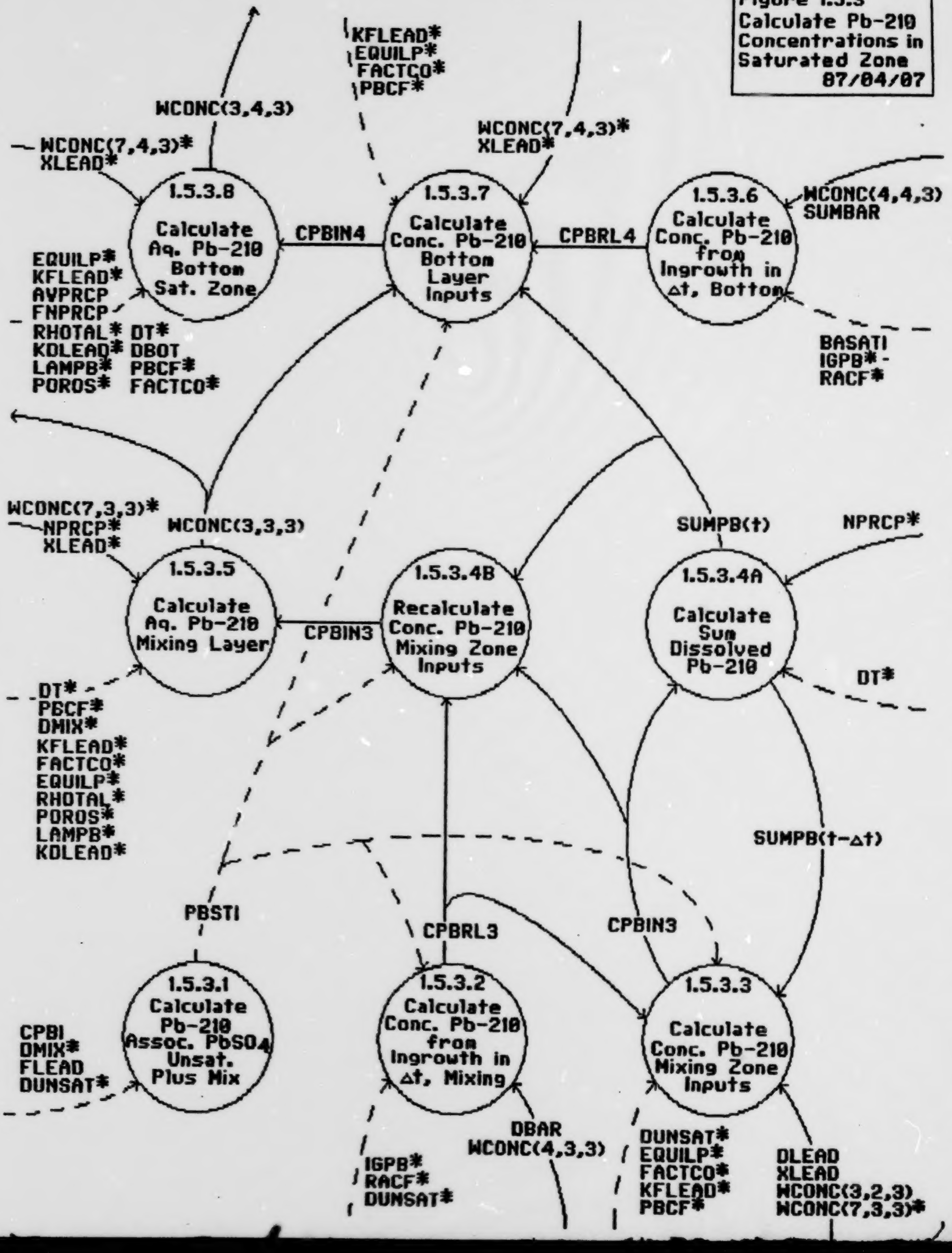

1.5.3.8
Calculate
Aq. Pb-210
Bottom
Sat. Zone
1.5.3.7
Calculate
Conc. Pb-210
Bottom
Layer
Inputs
1.5.3.6
Calculate
Conc. Pb-210
from
Ingrowth in
Δt, Bottom
1.5.3.5
Calculate
Aq. Pb-210
Mixing Layer
1.5.3.4B
Recalculate
Conc. Pb-210
Mixing Zone
Inputs
1.5.3.4A
Calculate
Sum
Dissolved
Pb-210
1.5.3.1
Calculate
Pb-210
Assoc. PbSO4
Unsat.
Plus Mix
1.5.3.2
Calculate
Conc. Pb-210
from
Ingrowth in
Δt, Mixing
1.5.3.3
Calculate
Conc. Pb-210
Mixing Zone
Inputs
WCONC(3,4,3)
KFLEAD*
EQUILP*
FACTCO*
PBCF*
WCONC(7,4,3)*
XLEAD*
WCONC(7,4,3)*
XLEAD*
WCONC(4,4,3)
SUMBAR
CPBIN4
CPBRL4
EQUILP*
KFLEAD*
AVPRCP
FNPRCP
RHOTAL*
KDLEAD*
LAMPB*
POROS*
DT*
DBOT
PBCF*
FACTCO*
BASATI
IGPB*
RACF*
WCONC(7,3,3)*
NPRCP*
XLEAD*
WCONC(3,3,3)
SUMPB(t)
NPRCP*
CPBIN3
DT*
DT*
PBCF*
DMIX*
KFLEAD*
FACTCO*
EQUILP*
RHOTAL*
POROS*
LAMPB*
KDLEAD*
SUMPB(t-Δt)
PBSTI
CPBRL3
CPBIN3
CPBI
DMIX*
FLEAD
DUNSAT*
DBAR
WCONC(4,3,3)
IGPB*
RACF*
DUNSAT*
DUNSAT*
EQUILP*
FACTCO*
KFLEAD*
PBCF*
DLEAD
XLEAD
WCONC(3,2,3)
WCONC(7,3,3)*

Figure 1.5.3.1
Calculate PB-210 ASSOC. PBSO4, UNSAT. PLUS MIX (PBSTI)

PBSTI - PB-210 ASSOC. PBSO4, UNSAT. PLUS MIX [mol m^{-2}]. The total lead-210 associated with $PbSO_4$ in the unsaturated and mixing zones of the tailings.

CPBI
DMIX
DUNSAT --- > PBSTI
FLEAD

Short Name	Long Name	SI Unit	Source
CPBI	INIT. SOLID PHASE CONC. PB-210 IN TAILINGS	[mol m^{-3}]	1.5.1.2
DMIX	THICKNESS OF MIXING ZONE	[m]	Sampled
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
FLEAD	FRACT. PB SOLUBLE	[-]	Sampled
PBSTI	PB-210 ASSOC. PBSO4, UNSAT. PLUS MIX	[mol m^{-2}]	1.5.3.1

$$PBSTI = CPBI * FLEAD * (DMIX + DUNSAT) \qquad \text{(See Note)}$$

Unit check

$$[mol\ m^{-3}] * [-] * ([m] + [m]) = [mol\ m^{-2}]$$

Note: No definition equation is given in SENES Vol. 3 (although a note on page 3-97 suggests it should have been defined in Section 3.7.4). The equation used is based on a letter from SENES (1986-12-02) which gives

$$M^\circ_{Pb} = X^\circ_{Pb-210/PbSO4} [PbSO_4]^\circ (\lambda_w + \lambda_{mix}).$$

Because $[Pb\text{-}210_s]^\circ_{PbSO4} = f_{Pb} [Pb\text{-}210_s]^\circ$ (eqn. 3.7.48)

and $X^\circ_{Pb-210/PbSO4} = [Pb\text{-}210_s]^\circ_{PbSO4} / [PbSO_4]^\circ$ (eqn. 3.7.50)

$M^\circ_{Pb} = [Pb\text{-}210_s]^\circ f_{Pb} (\lambda_w + \lambda_{mix})$ which is the equation used here.

CPBRL3 - CONC. PB-210 FROM INGROWTH IN ΔT, MIXING [mol m^{-3}]. The concentration of Pb-210 at the bottom of the mixing layer of the saturated zone resulting from ingrowth from dissolved Ra-226 during the time step Δt.

Figure 1.5.3.2
Calculate CONC. PB-210 FROM INGROWTH IN ΔT, MIXING (CPBRL3)

DUNSAT
IGPB - - - > CPBRL3 <——— DBAR
RACF WCONC(4,3,3)

Short Name	Long Name	SI Unit	Source
CPBRL3	CONC. PB-210 FROM INGROWTH IN ΔT, MIXING	[mol m^{-3}]	1.5.3.2
DBAR	THICKNESS BASO4 DEPLETED LAYER	[m]	1.4.2.4
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
IGPB	INGROWTH FACTOR FOR PB-210	[-]	1.5.1.1
RACF	CONVERSION FACTOR MOL TO BQ (RA-226)	[Bq mol^{-1}]	Sampled
WCONC(4,3,3)	AQ. RA IN MIXING LAYER	[Bq m^{-3}]	1.4.4.5

(a) if DBAR < DUNSAT
CPBRL3 = 0 (eqn. 3.11.9; see Note 1)

(b) if DBAR ≥ DUNSAT (eqn. 3.11.10; see Note 2)

$$\text{CPBRL3} = \frac{\text{WCONC}(4,3,3)*\text{IGPB}}{\text{RACF}}$$

Unit check

$$\text{(b)} \quad \frac{[\text{Bq m}^{-3}] * [-]}{[\text{Bq mol}^{-1}]} = [\text{mol m}^{-3}]$$

Note 1: Equation (3.11.9) uses "h_{Ra}" which is undefined elsewhere in the document; h_{Ra} is an error for h_{Ba} (DBAR) (SENES letter 1986-12-02).

Note 2: The factor RACF is required to convert the radium concentration, WCONC(4,3,3) from [Bq m^{-3}] to [mol m^{-3}].

Figure 1.5.3.3
Calculate CONC. PB-210
MIXING ZONE INPUTS
(CPBIN3)

CPBIN3 - CONC. PB-210 MIXING ZONE INPUTS [mol m^{-3}]
The concentration of lead-210 resulting from the various inputs to the mixing layer of the saturated zone.

PBCF				SUMPB(t-Δt)
EQUILP				DLEAD
KFLEAD	- - - >	CPBIN3	<———	XLEAD
FACTCO				WCONC(3,2,3)
DUNSAT				WCONC(7,3,3)
PBSTI				CPBRL3

Short Name	Long Name	SI Unit	Source
CPBIN3	CONC. PB-210 MIXING ZONE INPUTS	[mol m^{-3}]	1.5.3.3
CPBRL3	CONC. PB-210 FROM INGROWTH IN ΔT, MIXING	[mol m^{-3}]	1.5.3.2
DLEAD	THICKNESS PBSO4 DEPLETED LAYER	[m]	1.5.2.6
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
EQUILP	SQ. RT. EQBM. CONST. PBSO4	[mol m^{-3}]	1.5.2.1
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
KFLEAD	PBSO4(AQ) FORMATION CONSTANT	[m^3 mol^{-1}]	Sampled
PBCF	CONVERSION FACTOR MOL TO BQ (PB-210)	[Bq mol^{-1}]	Sampled
PBSTI	PB-210 ASSOC. PBSO4 UNSAT. PLUS MIX	[mol m^{-2}]	1.5.3.1
SUMPB	SUM DISSOLVED PB-210	[mol m^{-2}]	1.5.3.4A
WCONC(3,2,3)	AQ. PB-210 BOTTOM UNSAT. ZONE	[Bq m^{-3}]	1.5.2.7
WCONC(7,3,3)	CONC. OF SO4 AQ. IN MIXING LAYER	[mol m^{-3}]	1.1.4.6
XLEAD	MOLE FRACT. PB-210	[-]	1.5.2.3

(a) If SUMPB(t-Δt) $\geq$ PBSTI

$$\text{CPBIN3} = \text{CPBRL3} \qquad \text{(eqn. 3.11.16)}$$

(b) If SUMPB(t-Δt) < PBSTI and DLEAD < DUNSAT

$$\text{CPBIN3} = \frac{\text{WCONC(3,2,3)}}{\text{PBCF}} + \text{CPBRL3} \qquad \text{(eqn. 3.11.14)}$$

(c) If SUMPB(t-Δt) < PBSTI and DLEAD $\geq$ DUNSAT

$$\text{CPBIN3} = \left(\frac{\text{EQUILP*EQUILP*XLEAD}}{\text{EQUILP+WCONC(7,3,3)}}\right) * \left(1+\text{KFLEAD*(FACTCO)}^2\text{*WCONC(7,3,3)}\right) + \text{CPBRL3} \qquad \text{(eqn. 3.11.15)}$$

Unit check

(a) $[\text{mol m}^{-3}] = [\text{mol m}^{-3}]$

(b) $\dfrac{[\text{Bq m}^{-3}]}{[\text{Bq mol}^{-1}]} + [\text{mol m}^{-3}] = [\text{mol m}^{-3}]$

(c) $\left(\dfrac{[\text{mol m}^{-3}][\text{mol m}^{-3}][-]}{[\text{mol m}^{-3}] + [\text{mol m}^{-3}]}\right) * \left([-]+[\text{m}^3 \text{ mol}^{-1}][-]^2[\text{mol m}^{-3}]\right) + [\text{mol m}^{-3}] = [\text{mol m}^{-3}]$

Note 1: The initial condition is specified by use of equation (3.11.15) for the time interval between TIME=-Δt and TIME=0. Equation (3.7.53) is not used for layer 3 (SENES letter 1987-01-27).

Note 2: The factor PBCF is required to convert the Pb-210 concentration, WCONC(3,2,3)[Bq m^{-3}], to [mol m^{-3}].

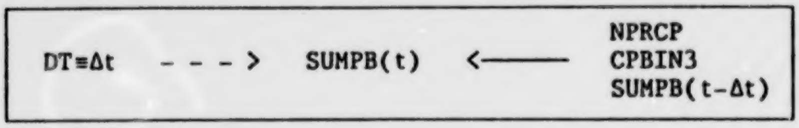
Note 3: Discussion of the inequalities is muddled in the text. Clarifications were made in a letter from SENES (1986-12-02).

Note 4: The assumption is made $[\text{Pb-210}_L]_{\lambda_W} \equiv [\text{Pb-210}]_{\lambda_W}$=WCONC(3,2,3) if all are converted to [Bq m^{-3}].

Note 5: SENES uses CPBIN to refer to Pb-210 inputs to the mixing zone and, later, to the bottom layer. We have used CPBIN3 and CPBIN4, respectively, to differentiate between these variables.

Figure 1.5.3.4A
Calculate
SUM DISSOLVED PB-210
(SUMPB)

SUMPB - SUM DISSOLVED PB-210 [mol m^{-2}].
Cumulative sum of lead-210 inputs to the mixing zone to TIME=t.



Short Name	Long Name	SI Unit	Source
CPBIN3	CONC. PB-210 MIXING ZONE INPUTS	[mol m^{-3}]	1.5.3.3
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled
SUMPB	SUM DISSOLVED PB-210	[mol m^{-2}]	1.5.3.4A

From the finite difference equation

$$SUMPB(t) = SUMPB(t-\Delta t) + NPRCP*CPBIN3*DT \qquad \text{(eqn. 3.11.7)}$$

with

$$SUMPB(-\Delta t) = 0 \qquad \text{(see Note 2)}$$

Unit check

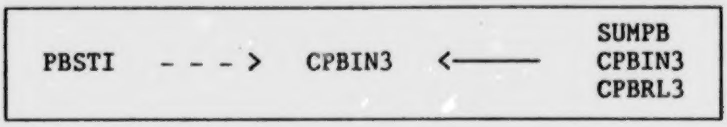
$$[mol\ m^{-2}] + [m\ a^{-1}] * [mol\ m^{-3}] * [a] \neq [mol\ m^{-3}]$$

Note 1: Unit check failure. SENES reports [mol m^{-3}] for SUMPB in Table A.3 but compares SUMPB with the (undefined) PBSTI [mol m^{-2}] (eqn. 3.11.18). [mol m^{-2}] is correct; SENES nomenclature is confusing (SENES letter 1986-12-02).

Note 2: The initial condition has been assumed (BWG, 87-03-23).

CPBIN3 - CONC. PB-210 MIXING ZONE INPUTS [mol m^{-3}]
The concentration of lead-210 resulting from the various inputs to the mixing layer of the saturated zone.

Figure 1.5.3.4B
Recalculate CONC.
PB-210 MIXING ZONE
INPUTS (CPBIN3)



Short Name	Long Name	SI Unit	Source
CPBIN3	CONC. PB-210 MIXING ZONE INPUTS	[mol m^{-3}]	1.5.3.3 & 1.5.3.4B
CPBRL3	CONC. PB-210 FROM INGROWTH IN Δt MIXING	[mol m^{-3}]	1.5.3.2
PBSTI	PB-210 ASSOC. PBSO4 UNSAT. PLUS MIX	[mol m^{-2}]	1.5.3.1
SUMPB	SUM DISSOLVED PB-210	[mol m^{-2}]	1.5.3.4A

a) If $SUMPB(t) \geq PBSTI$

$$CPBIN3 = CPBRL3 \qquad \text{(eqn. 3.11.16)}$$

b) else $CPBIN3 = CPBIN3$

Unit check:

$$[\text{mol m}^{-3}] = [\text{mol m}^{-3}]$$

Note: SENES uses CPBIN to refer to Pb-210 inputs to the mixing zone and, later, to the bottom layer. We have used CPBIN3 and CPBIN4, respectively, to differentiate between these values.

Figure 1.5.3.5
Calculate AQ. PB-210
MIXING LAYER
(WCONC(3,3,3))

WCONC(3,3,3) - AQ. PB-210 MIXING LAYER [Bq m^{-3}]. The concentration of lead-210 in the aqueous phase of the mixing layer of the saturated zone.

PBCF
LAMPB
EQUILP
DT≡Δt
POROS
DMIX
KFLEAD
KDLEAD
FACTCO
RHOTAL

- - -> WCONC(3,3,3) <——

WCONC(7,3,3)
CPBIN3
WCONC(3,3,2)
NPRCP
XLEAD

Short Name	Long Name	SI Unit	Source
CPBIN3	CONC. PB-210 MIXING ZONE INPUTS	[mol m^{-3}]	1.5.3.4B
DMIX	THICKNESS OF MIXING ZONE	[m]	Sampled
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
EQUILP	SQ. ROOT EQBM. CONST. $PBSO_4$	[mol m^{-3}]	1.5.2.1
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
KDLEAD	PB SOLID-LIQUID DISTR. COEFFICIENT	[m^3 g^{-1}]	Sampled
KFLEAD	$PBSO_4$(AQ) FORMATION CONSTANT	[m^3 mol^{-1}]	Sampled
LAMPB	PB-210 DECAY CONSTANT	[a^{-1}]	Sampled
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled
PBCF	CONVERSION FACTOR MOL TO BQ (PB-210)	[Bq mol^{-1}]	Sampled
POROS	TAILINGS POROSITY	[-]	Sampled
RHOTAL	TAILINGS BULK DENSITY	[g m^{-3}]	Sampled
WCONC(3,3,2)	AQ. PB-210 MIXING LAYER	[Bq m^{-3}]	(1.5.3.5)
WCONC(3,3,3)	AQ. PB-210 MIXING LAYER	[Bq m^{-3}]	1.5.3.5
WCONC(7,3,3)	CONC. OF SO_4 AQ. IN MIXING LAYER	[mol m^{-3}]	1.1.4.4
XLEAD	MOLE FRACT. PB-210	[-]	1.5.2.3

If t=0 then WCONC(3,3,3) = XLEAD * CLEADX * PBCF where (see Note 2)

$$\text{CLEADX} = (\text{EQUILP}^2/(\text{EQUILP} + \text{WCONC}(7,3,3)) * (1+\text{FACTCO}^2 * \text{KFLEAD} * \text{WCONC}(7,3,3))$$

Otherwise:

$$\text{WCONC}(3,3,3) = \text{PBCF}*\left\{\text{CPBIN3} + \left[\frac{\text{WCONC}(3,3,2)}{\text{PBCF}} * \text{EXP}\,[-\text{LAMPB}*\text{DT}] - \text{CPBIN3}\right] * \text{EXP}\left[\frac{-\text{NPRCP}*\text{DT}}{\text{POROS}*\text{DMIX}*\left(1 + \frac{\text{KDLEAD}*\text{RHOTAL}}{\text{POROS}}\right)}\right]\right\}$$

(eqn. 3.11.13; see Note 2)

Unit check

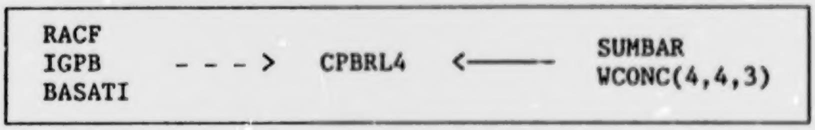
$$[\text{Bq mol}^{-1}] * \left\{[\text{mol m}^{-3}] + \left[\frac{[\text{Bq m}^{-3}]}{[\text{Bq mol}^{-1}]} * \text{EXP}([a^{-1}] * [a]) - [\text{mol m}^{-3}]\right] * \text{EXP}\left[\frac{-[\text{m a}^{-1}] * [a]}{[-] * [m] * \left(\frac{[-] + [\text{m}^3\text{g}^{-1}] * [\text{gm}^{-3}]}{[-]}\right)}\right]\right\} = [\text{Bq m}^{-3}]$$

Note 1: The factor PBCF is required so that WCONC(3,3,3) is in units of [Bq m^{-3}].

Note 2: Initial condition deduced from an inspection of the UTAP2 code (BWG, 87-04-02).

Figure 1.5.3.6
Calculate CONC. PB-210
FROM INGROWTH IN ΔT,
BOTTOM (CPBRL4)

CPBRL4 - CONC. PB-210 FROM INGROWTH IN ΔT, BOTTOM [mol m^{-3}]. The concentration of Pb-210 in the bottom layer of the saturated zone resulting from ingrowth from dissolved Ra-226 during the time step Δt.



Short Name	Long Name	SI Unit	Source
BASATI	INIT. RA ASSOC. BA UNSAT. PLUS MIX	[mol m^{-2}]	1.4.4.1
CPBRL4	CONC. PB-210 FROM INGROWTH IN ΔT, BOTTOM	[mol m^{-3}]	1.5.3.6
IGPB	INGROWTH FACTOR FOR PB-210	[-]	1.5.1.1
RACF	CONVERSION FACTOR MOL TO BQ (RA-226)	[Bq mol^{-1}]	Sampled
SUMBAR	SUM DISSOLVED RA	[mol m^{-2}]	1.4.4.4
WCONC(4,4,3)	AQ. RA IN BOTTOM SAT. ZONE	[Bq m^{-3}]	1.4.4.8

a) if SUMBAR < BASATI

$$\text{CPBRL4} = 0. \qquad \text{(eqn. 3.11.11)}$$

b) if SUMBAR ≥ BASATI

$$\text{CPBRL4} = \frac{\text{WCONC(4,4,3)} * \text{IGPB}}{\text{RACF}} \qquad \text{(eqn. 3.11.12)}$$

Unit check

b) $$\frac{[\text{Bq m}^{-3}] * [-]}{[\text{Bq mol}^{-1}]} = [\text{mol m}^{-3}]$$

Note 1: The factor RACF is required to convert the radium concentration, WCONC(4,4,3)[Bq m^{-3}], to [mol m^{-3}]. Furthermore, the factor IGPB, defined in Figure 1.5.1.1 has been used to modify (simplify) equation (3.11.12).

Note 2: WCONC(4,4,3) = $[Ra_L]_4$ (SENES letter 1987-02-03).

Figure 1.5.3.7
Calculate CONC. PB-210
BOTTOM LAYER INPUTS
(CPBIN4)

CPBIN4 - CONC. PB-210 BOTTOM LAYER INPUTS [mol m^{-3}]. The concentration of lead-210 resulting from the various inputs to the bottom layer of the saturated zone.

FACTCO PBCF EQUILP KFLEAD PBSTI	- - - >	CPBIN4	<———	SUMPB XLEAD WCONC(3,3,3) WCONC(7,4,3) CPBRL4

Short Name	Long Name	SI Unit	Source
CPBIN4	CONC. PB-210 BOTTOM LAYER INPUTS	[mol m^{-3}]	1.5.3.7
CPBRL4	CONC. PB-210 FROM INGROWTH IN Δt, BOTTOM	[mol m^{-3}]	1.5.3.6
EQUILP	SQ. ROOT OF EQBM. CONST. PBSO4	[mol m^{-3}]	1.5.2.1
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
KFLEAD	PBSO4(AQ) FORMATION CONSTANT	[m^3 mol^{-1}]	Sampled
PBCF	CONVERSION FACTOR MOL TO BQ (PB-210)	[Bq mol^{-1}]	Sampled
PBSTI	PB-210 ASSOC. PBSO4 UNSAT. PLUS MIX	[mol m^{-2}]	1.5.3.1
SUMPB	SUM DISSOLVED PB-210	[mol m^{-2}]	1.5.3.4
WCONC(3,3,3)	AQ. PB-210 MIXING LAYER	[Bq m^{-3}]	1.5.3.5
WCONC(7,4,3)	CONC. OF SO4 AQ. IN BOTTOM LAYER	[mol m^{-3}]	1.1.5.3
XLEAD	MOLE FRACT. PB-210	[-]	1.5.2.3

(a) if SUMPB < PBSTI

$$\text{CPBIN4} = \frac{\text{WCONC(3,3,3)}}{\text{PBCF}} + \text{CPBRL4} \qquad \text{(eqn. 3.11.20)}$$

(b) if SUMPB ≥ PBSTI

$$\text{CPBIN4} = \left(\frac{\text{EQUILP*EQUILP*XLEAD}}{\text{EQUILP+WCONC(7,4,3)}}\right)$$

$$* \ [(1+\text{KFLEAD}*(\text{FACTCO})^2*\text{WCONC(7,4,3)}] + \text{CPBRL4} \qquad \text{(eqn. 3.11.21)}$$

Unit check

(a) $$\frac{[\text{Bq m}^{-3}]}{[\text{Bq mol}^{-1}]} + [\text{mol m}^{-3}] = [\text{mol m}^{-3}]$$

(b) $$\left(\frac{[\text{mol m}^{-3}]*[\text{mol m}^{-3}]*[-]}{[\text{mol m}^{-3}]+[\text{mol m}^{-3}]}\right)*\left([-]+[\text{m}^3 \text{ mol}^{-1}]*[-]^2*[\text{mol m}^{-3}]\right)+[\text{mol m}^{-3}]=[\text{mol m}^{-3}]$$

Note 1: The factor PBCF is required to convert the Pb-210 concentration, WCONC(3,3,3) [Bq m^{-3}], to [mol m^{-3}].

Note 2: Discussion of the inequalities is muddled in the text. A SENES letter (1986-12-02) provides clarification.

Note 3: EQUILP, defined near equation (3.11.4), has been used to modify (simplify) equation (3.11.21).

Note 4: SENES used CPBIN for Pb-210 inputs to the mixing layer and, later, to the bottom layer. We have used CPBIN3 and CPBIN4 to differentiate between these variables.

Note 5: The initial condition is specified by the use of equation (3.11.21) for the time interval between TIME=-Δt and TIME=0. Equation (3.7.53) is not used for layer 4 (SENES letter 1987-01-27).

WCONC(3,4,3) - AQ. PB-210 BOTTOM SAT. ZONE [Bq m^{-3}]. The concentration of lead-210 in the aqueous phase in the bottom layer of the saturated zone.

Figure 1.5.3.8
Calculate AQ. PB-210
BOTTOM SAT. ZONE
WCONC(3,4,3)

$$\begin{tikzcd} \begin{array}{l}\text{PBCF}\\ \text{EQUILP}\\ \text{LAMPB}\\ \text{DT}\equiv\Delta\text{T}\\ \text{FACTCO}\\ \text{POROS}\\ \text{KFLEAD}\\ \text{DBOT}\\ \text{AVPRCP}\\ \text{KDLEAD}\\ \text{RHOTAL}\\ \text{FNPRCP}\end{array} \arrow[r, dashed] & \text{WCONC(3,4,3)} & \begin{array}{l}\text{CPBIN4}\\ \text{WCONC(3,4,2)}\\ \text{WCONC(7,4,3)}\\ \text{XLEAD}\end{array} \arrow[l] \end{tikzcd}$$

Short Name	Long Name	SI Unit	Source
AVPRCP	AVERAGE NET PRECIPITATION	[m a^{-1}]	Sampled
CPBIN4	CONC. PB-210 BOTTOM LAYER INPUTS	[mol m^{-3}]	1.5.3.7
DBOT	THICKNESS LAYER 4	[m]	1.1.1.4
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
EQUILP	SQ. ROOT OF EQBM. CONST. PBSO4	[mol m^{-3}]	1.5.2.1
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS	[-]	Sampled
FNPRCP	FRACT. NET PRECIP.	[-]	Sampled
KDLEAD	PB SOLID-LIQUID DISTR. COEFFICIENT	[m^3 g^{-1}]	Sampled
KFLEAD	PBSO$_4$(AQ) FORMATION CONSTANT	[m^3 mol^{-1}]	Sampled
LAMPB	PB-210 DECAY CONSTANT	[a^{-1}]	Sampled
PBCF	CONVERSION FACTOR MOL TO BQ (PB-210)	[Bq mol^{-1}]	Sampled
POROS	TAILINGS POROSITY	[-]	Sampled
RHOTAL	TAILINGS BULK DENSITY	[g m^{-3}]	Sampled
WCONC(3,4,2)	AQ. PB-210 BOTTOM SAT. ZONE	[Bq m^{-3}]	(1.5.3.8)
WCONC(3,4,3)	AQ. PB-210 BOTTOM SAT. ZONE	[Bq m^{-3}]	1.5.3.8
WCONC(7,4,3)	CONC. OF SO$_4$ AQ. IN BOTTOM LAYER	[mol m^{-3}]	1.1.5.3
XLEAD	MOLE FRACT. PB-210	[-]	1.5.2.3

If t=0 then WCONC(3,4,3) = XLEAD * CLEADX * PBCF where (see Note 2)

$$\text{CLEADX} = (\text{EQUILP} **2/(\text{EQUILP} + \text{WCONC}(7,4,3)) * (1 + \text{FACTCO}^2 * \text{KFLEAD} * \text{WCONC}(7,4,3))$$

Otherwise:

$$\text{WCONC}(3,4,3) = \text{PBCF}*\left\{\text{CPBIN4} + \left[\frac{\text{WCONC}(3,4,2)}{\text{PBCF}} * \text{EXP}[-\text{LAMPB}*\text{DT}] - \text{CPBIN4}\right] * \text{EXP}\left[\frac{-\text{FNPRCP}*\text{AVPRCP}*\text{DT}}{\text{POROS}*\text{DBOT}*\left(1+\frac{\text{KDLEAD}*\text{RHOTAL}}{\text{POROS}}\right)}\right]\right\}$$

(eqn. 3.11.19; see Note 2)

Unit check:

$$[\text{Bq mol}^{-1}] * \left\{[\text{mol m}^{-3}]+\left[\frac{[\text{Bq m}^{-3}]}{[\text{Bq mol}^{-1}]}*\text{EXP}([\text{a}^{-1}]*[\text{a}])-[\text{mol m}^{-3}]\right] * \text{EXP}\left[\frac{[-]*[\text{m a}^{-1}]*[\text{a}]}{[-]*[\text{m}]*\left([-]+\frac{[\text{m}^3\ \text{g}^{-1}]*[\text{g m}^{-3}]}{[-]}\right)}\right]\right\} = [\text{Bq m}^{-3}]$$

Note 1: The factor PBCF is required so that WCONC(3,4,3) is in units of [Bq m^{-3}].

Note 2: Initial condition deduced from an inspection of the UTAP2 code. (PWG, 87-04-02)

Note 3: See also response #81 in Appendix A.

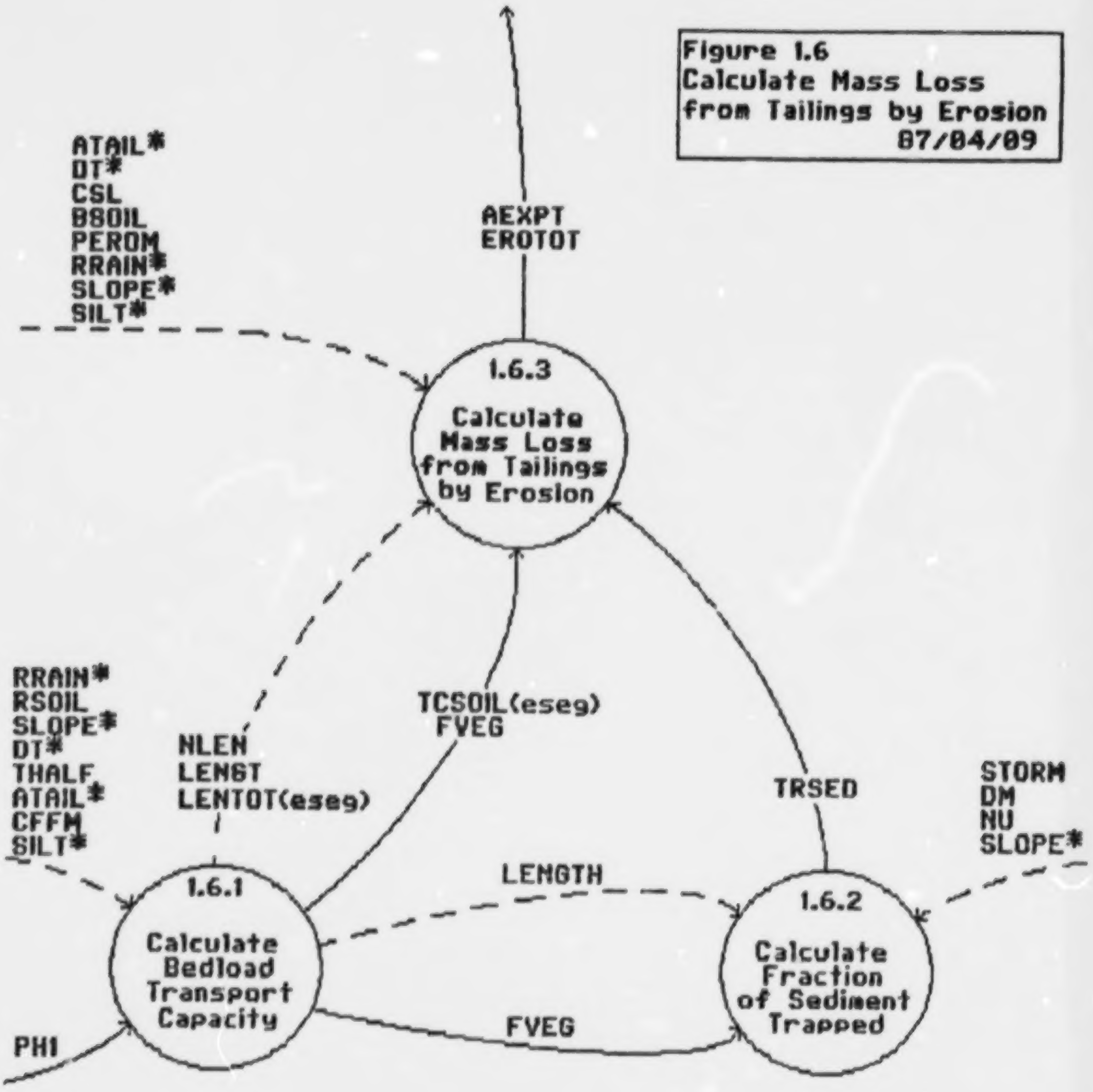


Figure 1.6
Calculate Mass Loss
from Tailings by Erosion
87/04/09

ATAIL*
DT*
CSL
BSOIL
PEROM
RRAIN*
SLOPE*
SILT*
AEXPT
EROTOT
1.6.3
Calculate Mass Loss from Tailings by Erosion
RRAIN*
RSOIL
SLOPE*
DT*
THALF
ATAIL*
CFFM
SILT*
NLEN
LENGT
LENTOT(eseg)
TCSOIL(eseg)
FVEG
TRSED
STORM
DM
NU
SLOPE*
LENGTH
1.6.1
Calculate Bedload Transport Capacity
1.6.2
Calculate Fraction of Sediment Trapped
PHI
FVEG

Figure 1.6.1
Calculate Bedload
Transport Capacity
87/04/10

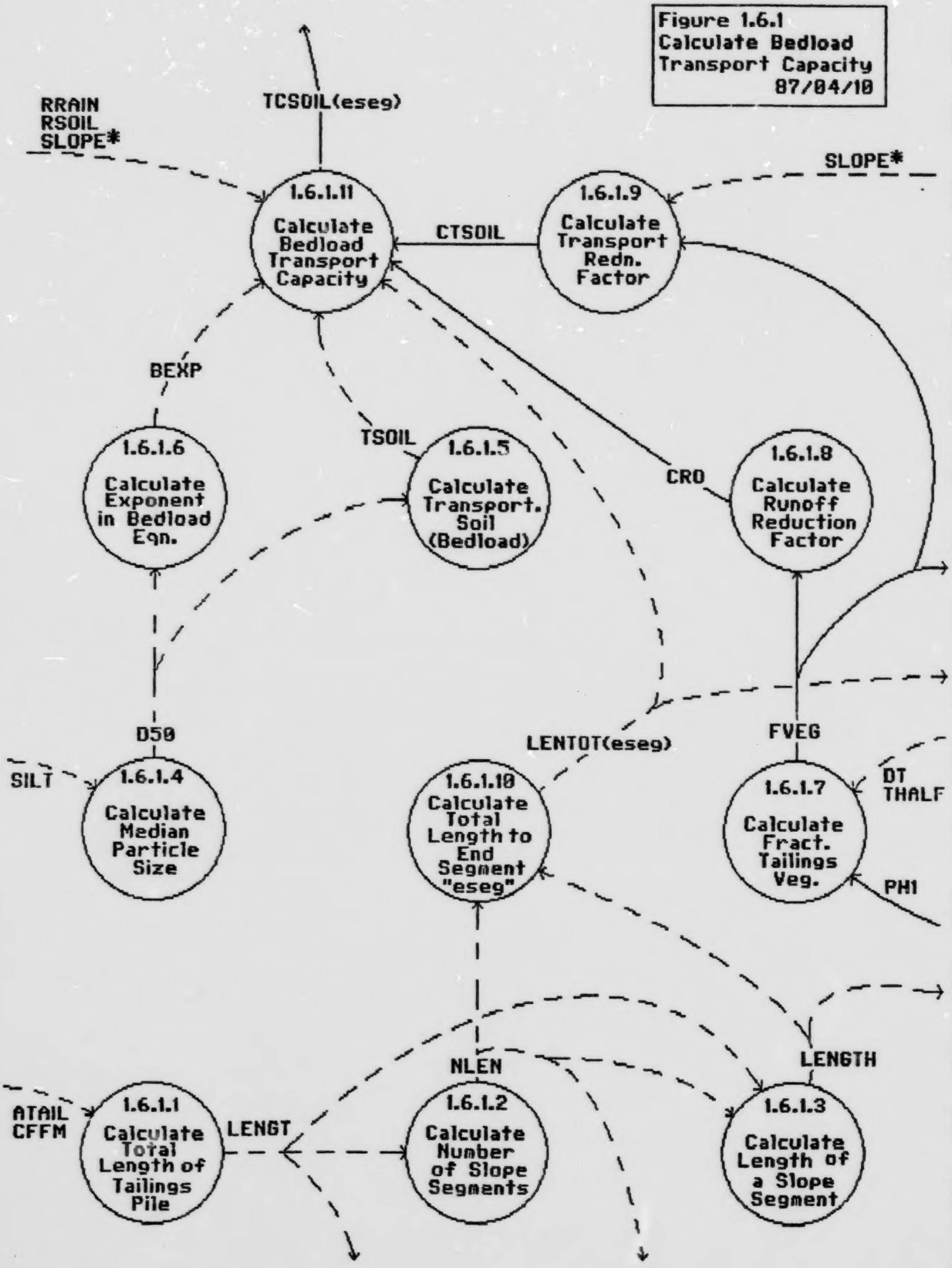

TCSOIL(eseg)
RRAIN
RSOIL
SLOPE*
1.6.1.11
Calculate Bedload Transport Capacity
CTSOIL
SLOPE*
1.6.1.9
Calculate Transport Redn. Factor
BEXP
TSOIL
1.6.1.6
Calculate Exponent in Bedload Eqn.
1.6.1.5
Calculate Transport. Soil (Bedload)
CRO
1.6.1.8
Calculate Runoff Reduction Factor
D50
LENTOT(eseg)
FVEG
SILT
1.6.1.4
Calculate Median Particle Size
1.6.1.10
Calculate Total Length to End Segment "eseg"
DT
THALF
1.6.1.7
Calculate Fract. Tailings Veg.
PH1
LENGTH
NLEN
ATAIL
CFFM
1.6.1.1
Calculate Total Length of Tailings Pile
LENGT
1.6.1.2
Calculate Number of Slope Segments
1.6.1.3
Calculate Length of a Slope Segment

Figure 1.6.1.1
Calculate TOTAL LENGTH OF TAILINGS PILE (LENGT)

LENGT - TOTAL LENGTH OF TAILINGS PILE [ft].
The total length of the slope of the tailings pile.

$$\begin{matrix} \text{ATAIL} \\ \text{CFFM} \end{matrix} \dashrightarrow \text{LENGT}$$

Short Name	Long Name	SI Unit	Source
ATAIL	INITIAL EXPOSED TAILINGS SURFACE AREA	$[m^2]$	Sampled
CFFM	CONVERSION FACTOR FEET TO METERS	$[m\ ft^{-1}]$	Sampled
LENGT	TOTAL LENGTH OF TAILINGS PILE	[ft]	1.6.1.1

$$\text{LENGT} = \left(\frac{\sqrt{\text{ATAIL}}}{\text{CFFM}} \right)$$

(bottom page 3-124 and SENE letter 1987-01-13, reply to question 76)

Unit check:

$$\frac{[m^2]^{0.5}}{[m\ ft^{-1}]} = [ft]$$

Note: The factor CFFM was supplied by SENES in a letter 1987-01-13 (see reply to question 76).

NLEN - NUMBER OF SLOPE SEGMENTS [-].
The maximum number of equal-length segments, each less than 400 ft, into which the tailings pile is subdivided for the purpose of calculating erosion losses.

Figure 1.6.1.2
Calculate NUMBER OF
SLOPE SEGMENTS
(NLEN)

LENGT - - -> NLEN

Short Name	Long Name	SI Unit	Source
LENGT	TOTAL LENGTH OF TAILINGS PILE	[ft]	1.6.1.1
NLEN	NUMBER OF SLOPE SEGMENTS	[-]	1.6.1.2

$$\text{NLEN} = \text{INTEGER PART OF } \left(\frac{\text{LENGT}}{400}\right) + 1$$

(bottom of page 3-124) and (SENES letter 1987-01-13, reply to question 76)

Unit check:

$$\left(\text{INT}\left(\frac{[\text{ft}]}{[\text{ft}]}\right) + [-]\right) = [-]$$

Note: The 400 has units [ft]. It is assumed that the "1" is added to ensure the segments have a maximum size of 400 [ft] when an integral number of equal-length segments are used. The "1" is also assumed to be dimensionless.

LENGTH - LENGTH OF A SLOPE SEGMENT [ft].
The length of each segment of the tailings pile such that there is a minimum number of equal-length segments each less than 400 ft in length.

Figure 1.6.1.3
Calculate LENGTH OF
A SLOPE SEGMENT
(LENGTH)

NLEN
LENGT - - -> LENGTH

Short Name	Long Name	SI Unit	Source
LENGT	TOTAL LENGTH OF TAILINGS PILE	[ft]	1.6.1.1
LENGTH	LENGTH OF A SLOPE SEGMENT	[ft]	1.6.1.3
NLEN	NUMBER OF SLOPE SEGMENTS	[-]	1.6.1.2

$$\mathrm{LENGTH} = \frac{\mathrm{LENGT}}{\mathrm{NLEN}}$$

(see Note)

Unit check:

$$\frac{[\mathrm{ft}]}{[-]} = [\mathrm{ft}]$$

Note: From the discussion at the bottom of SENES Vol. 3 pg 3-124 and information in a letter (1987-01-13, reply to question 76) from SENES.

D50 - MEDIAN PARTICLE SIZE [mm].
The particle diameter size exceeded by only 50% of the tailings particles.

Figure 1.6.1.4
Calculate MEDIAN PARTICLE SIZE (D50)

SILT - - -> D50

Short Name	Long Name	SI Unit	Source
D50	MEDIAN PARTICLE SIZE	[mm]	1.6.1.4
SILT	SILT CONTENT OF TAILINGS SURFACE	[%]	Sampled

$$D50 = -1.99 \times 10^{-3} * SILT + 0.215 \qquad \text{(eqn. 3.14.10)}$$

Unit check:

[mm] [-] + [mm] = [mm]

Note: Units of [mm] have been assumed for -1.99×10^{-3} and 0.215 in order to make units consistent with those indicated for equation (3.14.11).

Figure 1.6.1.5
Calculate TRANSPORT. SOIL (BEDLOAD) (TSOIL)
and
Figure 1.6.1.6
Calculate EXPONENT IN BEDLOAD EQN. (BEXP)

TSOIL - TRANSPORT. SOIL (BEDLOAD) [lb s^{-1} ft^{-5}]. A parameter representing the transportability of soil particles in bedload transport.

BEXP - EXPONENT IN BEDLOAD EQN. [-]. An empirical exponent used in the bedload transport capacity equation.

D50 - - -> BEXP

D50 - - -> TSOIL

Short Name	Long Name	SI Unit	Source
BEXP	EXPONENT IN BEDLOAD EQN.	[-]	1.6.1.6
D50	MEDIAN PARTICLE SIZE	[mm]	1.6.1.4
TSOIL	TRANSPORT. SOIL (BEDLOAD)	[lb s^{-1} ft^{-5})	1.6.1.5

$$\text{TSOIL} = 5.87\text{x}10^5 * \left(\frac{D_{50}}{1}\right)^{0.197}$$ (eqn. 3.14.9)

If $0.016 \leq \text{D50} < 0.045$

$$\text{BEXP} = 1.83 * \left(\left(\frac{\text{D50}}{1}\right) * \text{EXP}(0.049)\right)$$

(eqn. 3.14.11 modified in SENES letter (1987-01-27); see Note 3)

If $0.045 \leq \text{D50} \leq 0.215$

$$\text{BEXP} = -0.714 * \left(\frac{\text{D50}}{1}\right) + 1.61$$

Unit check:

$$\text{TSOIL } [\text{lb s}^{-1} \text{ ft}^{-5}] \left(\frac{[\text{mm}]}{[\text{mm}]}\right)^{0.197} = [\text{lb s}^{-1} \text{ ft}^{-5}]$$

$$\text{BEXP} \qquad [-] * \left(\frac{[\text{mm}]}{[\text{mm}]}\right) = [-]$$

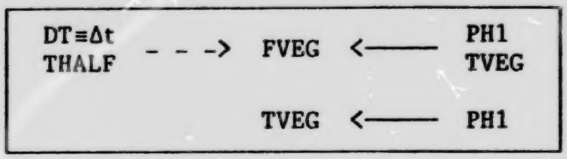
Note 1: Both equations 3.14.9 and 3.14.11 have been modified by replacing by replacing D50 by $\left(\frac{\text{D50}}{1}\right)$ with "1" having dimensions of mm. This allows consistency of units to be maintained.

Note 2: Units of 5.87 x 10^5 assumed [lb s^{-1} ft^{-5}] to agree with TSOIL (SENES letter 1987-01-13, reply number 73).

Note 3: Inspection of the UTAP2 code shows that the equation for D50 is
if D50<0.045 then BEXP = $1.83\text{xD50}^{0.49}$
otherwise BEXP = -0.714*D50+1.61.
SYVAC3-UT2 has been changed accordingly. (BWG, 87-04-10)

FVEG - FRACT. TAILINGS VEG. [-].
Fraction of the surface area of the tailings pile that is vegetated.

Figure 1.6.1.7
Calculate FRACT. TAILINGS VEG. (FVEG)
(Page 1 of 2)



Short Name	Long Name	SI Unit	Source
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
FVEG	FRACT. TAILINGS VEG.	[-]	1.6.1.7
PH1	PH LAYER 1	[-]	1.1.3.2
THALF	REVEG. HALF LIFE	[a]	Sampled
TVEG	TIME VEG. BEGINS	[a]	---

(a) If $\text{TIME} \leq 0$
$\text{TVEG} = 0$

(b) If $\text{PH1}(t-\Delta t) \leq 4.0$
$\text{TVEG} = \text{TIME}$

(c) If $\text{PH1}(t-\Delta t) > 4$
and $\text{PH1}(t) > 4$
$\text{TVEG} = \text{TVEG}$

(discussion above eqn. 3.14.7 and SENES letter 1987-01-13, reply to questions 72 and 76)

(a) If $\text{TVEG} = \text{TIME}$
$\text{FVEG} = 0$

(SENES letter 1987-01-13, replies 72 and 76)

(b) If $\text{TVEG} < \text{TIME}$

$$\text{FVEG} = 1-\text{EXP}\left(\left(\frac{-\ln 2}{\text{THALF}}\right) * \left((\text{TIME}-\text{TVEG}) - \frac{\text{DT}}{2.0}\right)\right)$$

(eqn. 3.14.7; see Note 3)

(c) If $\text{FVEG} > 0.9$ $\quad \text{FVEG} = 0.9$

(SENES, letter 1987-01-13, replies 72 and 76)

Unit check:

$\text{TVEG} \quad [a] = [a]$

$$\text{FVEG (b)} \quad [-] - \text{EXP}\left(\frac{[-]}{[a]} * \left(([a]-[a]) - \frac{[a]}{[-]}\right)\right) = [-]$$

Note 1: If pH1 is > 4 at $t=-\Delta t$ and at $t=0$ revegetation does not begin until $t=0$ (SENES letter 1987-01-13).

Note 2: The values "1" and "2" in equation (3.14.7) are assumed dimensionless.

Figure 1.6.1.7
Calculate FRACT.
TAILINGS VEG.
(FVEG)
(Page 2 of 2)

Note 3: Equation (3.14.7) has been modified according to a letter from SENES (1987-01-13), replies 72 and 76.

Note 4: Inspection of the UTAP2 code shows some inconsistency with the above equations. We have implemented the UTAP2 logic, which is as follows:

(a) If t=0 then TVEG=-1.

(b) If PH1 $\leq$ 4 then FVEG=0 and CSOIL=1

    Otherwise if TVEG=-1 then TVEG=T and FVEG=0

        otherwise $\text{FVEG} = 1\text{-EXP}\left[\frac{-0.693}{\text{THALF}} * (\text{T-TVEG-}\frac{\text{DT}}{2})\right]$

        if FVEG>0.9 then FVEG=0.9

        CSOIL=EXP[-0.109-(0.0506*FVEG)]

Condition (b) is applicable after condition (a), and the indented statements imply logic flows. (BWG, 87-04-10)

Figure 1.6.1.8
Calculate RUNOFF
REDUCTION FACTOR
(CRO)
and
Figure 1.6.1.9
Calculate TRANSPORT.
REDN. FACTOR
(CTSOIL)

CRO - RUNOFF REDUCTION FACTOR [-].
Runoff reduction factor used in the bedload transport capacity equation.

CTSOIL - TRANSPORT. REDN. FACTOR [-].
The transportability reduction factor used in the bedload transport capacity equation (given as a function of velocity with respect to bare soil for several slopes).

CRO <—— FVEG
SLOPE - - -> CTSOIL <—— VELRAT
VELRAT <—— FVEG

Short Name	Long Name	SI Unit	Source
CRO	RUNOFF REDUCTION FACTOR	[-]	1.6.1.8
CTSOIL	TRANSPORT. REDN. FACTOR	[-]	1.6.1.9
FVEG	FRACT. TAILINGS VEG.	[-]	1.6.1.7
SLOPE	TAILINGS SLOPE	[-]	Sampled
VELRAT	VELOC. RATIO (BEDLOAD)	[-]	(1.6.1.9)

$$\text{CRO} = -1.44 * \text{FVEG} + 1.4 \qquad \text{(eqn. 3.14.12)}$$

$$\text{VELRAT} = -0.77 * \text{FVEG} + 1.0 \qquad \text{(eqn. 3.14.13)}$$

If $\text{SLOPE} > 1.5$
$\text{CTSOIL} = 1.08 * \text{VELRAT}^{6.7}$

If $0.75 < \text{SLOPE} \leq 1.5$
$\text{CTSOIL} = 1.12 * \text{VELRAT}^{9.27}$

If $\text{SLOPE} \leq 0.75$
$\text{CTSOIL} = 1.14 * \text{VELRAT}^{18.98}$

(eqn. 3.14.14, as modified by SENES in a letter dated 1987-01-13, response 76)

Unit check:
CRO: [-] * [-] + [-] = [-]
VELRAT: [-] * [-] + [-] = [-]
CTSOIL: $[-] * [-]^{n} = [-]$

Note: All numbers were assumed dimensionless in equations (3.14.12), (3.14.13) and (3.14.14).

LENTOT(eseg) - TOTAL LENGTH TO END SEGMENT "eseg" [ft]. The total length of the slope of the tailings pile from the top to the bottom of segment "eseg".

Figure 1.6.1.10
Calculate TOTAL LENGTH TO END SEGMENT "eseg" (LENTOT(eseg))

LENGTH
NLEN
- - -> LENTOT(eseg)

Short Name	Long Name	SI Unit	Source
LENGTH	LENGTH OF A SLOPE SEGMENT	[ft]	1.6.1.3
LENTOT(eseg)	TOTAL LENGTH TO END SEGMENT "eseg"	[ft]	1.6.1.10
NLEN	NUMBER OF SLOPE SEGMENTS	[-]	1.6.1.2

for eseg = 1, NLEN

LENTOT(eseg) = LENGTH * eseg

(SENES letter
1987-01-13,
response 76)

Unit check:
[-] * [ft] = [ft]

Note: "eseg" is a dimensionless index representing the slope segment number.

Figure 1.6.1.11
Calculate SEGMENT BEDLOAD TRANSPORT CAPACITY (TCSOIL(eseg))

TCSOIL(eseg) - SEGMENT BEDLOAD TRANSPORT CAPACITY [lb ft^{-1} a^{-1}]. Bedload transport capacity of the tailings for the j^{th} segment.

```
RRAIN
RSOIL
TSOIL                                       CTSOIL
BEXP          - - ->  TCSOIL(eseg)  <-----  CRO
SLOPE
LENTOT(eseg)
```

Short Name	Long Name	SI Unit	Source
BEXP	EXPONENT IN BEDLOAD EQN.	[-]	1.6.1.6
CRO	RUNOFF REDUCTION FACTOR	[-]	1.6.1.8
CTSOIL	TRANSPORT. REDN. FACTOR	[-]	1.6.1.9
LENTOT(eseg)	TOTAL LENGTH TO END SEGMENT "eseg"	[ft]	1.6.1.10
RRAIN	RAINFALL EROS. FACTOR	[100(ft tons $acre^{-1}$)(in hr.)]	Sampled
RSOIL	BEDLOAD TRANSPORT EQN. CONST.	[ft^2 s^{-1} a^{-1} (units of RRAIN)]	"
SLOPE	TAILINGS SLOPE	[-]	Sampled
TCSOIL(eseg)	SEGMENT BEDLOAD TRANSPORT CAPACITY	[lb ft^{-1} a^{-1}]	1.6.1.11
TSOIL	TRANSPORT. SOIL (BEDLOAD)	[lb s^{-1} ft^{-5}]	1.6.1.5

for eseg = 1, NLEN

$$\text{TCSOIL(eseg)} = \text{RSOIL} * \text{RRAIN} * \text{TSOIL} * (\text{LENTOT(eseg)})^2 * \left\{ \text{SIN} \left(\text{ATAN} \left(\frac{\text{SLOPE}}{100} \right) \right) \right\}^{\text{BEXP}} * \text{CRO} * \text{CTSOIL}$$

(eqn. 3.14.8, as modified by a letter from SENES 87-01-13, response 73)

Unit check:

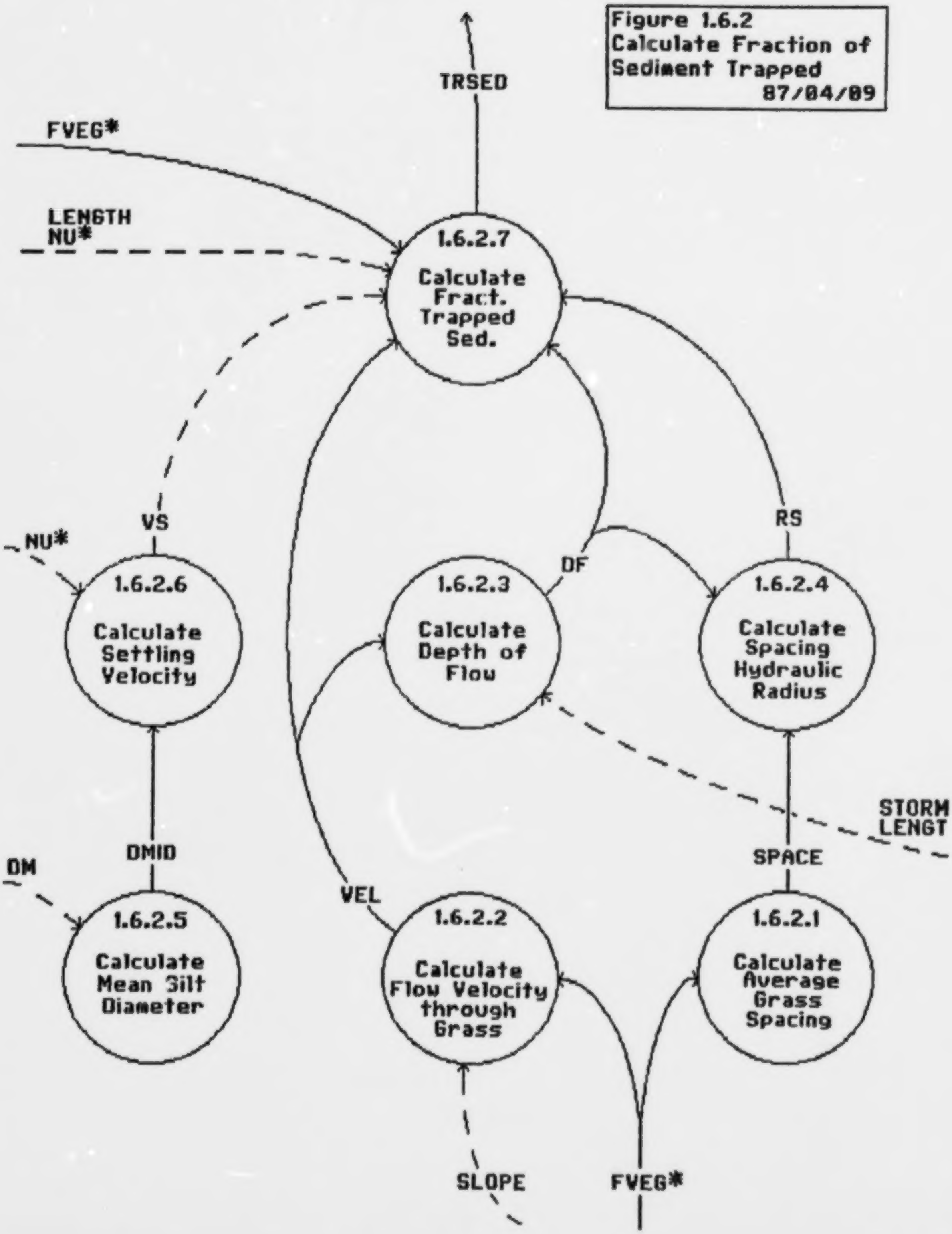
$$[ft^2\ s^{-1}\ a^{-1}\ (\text{units of RRAIN})^{-1}] * [\text{units of RRAIN}] * [lb\ s\ ft^{-5}] * [ft]^2 * [-] * [-] * [-] = [lb\ ft^{-1}\ a^{-1}]$$

Note 1: Unit check failure corrected in letter from SENES (1987-01-13), response #73, for units of RRAIN (see DD).

Note 2: SLOPE is defined as the "percentage slope" and, therefore, the tangent of the slope angle is SLOPE/100 (SENES letter 1987-01-13).

Note 3: The meaning of the terms in equation (3.14.8), especially with respect to LENTOT, was clarified in a letter from SENES (1987-01-13), responses #73 and 76. The definition of "x" in eqn. (3.14.8) is given below eqn. (3.4.3) and in response #70 of the SENES letter.

Figure 1.6.2
Calculate Fraction of Sediment Trapped
87/04/09


TRSED
FVEG*
LENGTH
NU*
1.6.2.7
Calculate Fract. Trapped Sed.
VS
RS
NU*
DF
1.6.2.6
Calculate Settling Velocity
1.6.2.3
Calculate Depth of Flow
1.6.2.4
Calculate Spacing Hydraulic Radius
STORM
LENGT
DMID
SPACE
DM
VEL
1.6.2.5
Calculate Mean Silt Diameter
1.6.2.2
Calculate Flow Velocity through Grass
1.6.2.1
Calculate Average Grass Spacing
SLOPE
FVEG*

SPACE - AVERAGE GRASS SPACING [ft].
The average spacing of grass as vegetation.

VEL - FLOW VELOCITY THROUGH GRASS [ft s^{-1}].
Flow velocity through grass calculated as a function of tailings slope.

Figure 1.6.2.1
Calculate AVERAGE GRASS SPACING (SPACE)
and
Figure 1.6.2.2
Calculate FLOW VELOCITY THROUGH GRASS (VEL)

SPACE <—— FVEG

SLOPE - - -> VEL <—— FVEG

Short Name	Long Name	SI Unit	Source
FVEG	FRACT. TAILINGS VEG.	[-]	1.6.1.7
SLOPE	TAILINGS SLOPE	[-]	Sampled
SPACE	AVERAGE GROSS SPACING	[ft]	1.6.2.1
VEL	FLOW VELOCITY THROUGH GRASS	[ft s^{-1}]	1.6.2.2

If FVEG = 0

$$VEL = EXP(-0.394 + 0.276 * SLOPE) \quad \text{(eqn. 3.14.17)}$$

If FVEG > 0

$$VEL = EXP(-0.905 + 0.503 * SLOPE) \quad \text{(eqn. 3.14.18)}$$

$$SPACE = -0.034 * FVEG + 0.056 \quad \text{(eqn. 3.14.19)}$$

Unit check:

VEL: $EXP([-] + [-] * [-]) \neq [ft\ s^{-1}]$ (see Note 1)

SPACE: $[ft] * [-] + [ft] = [ft]$ (see Note 2)

Note 1: If VEL has units of [ft s^{-1}] (SENES pg. 3-128) then the expressions given by equations (3.14.17) and (3.14.18) must be multiplied by a factor of 1 [ft s^{-1}]. It is also assumed that the constants in eqns. (3.14.17) and (3.14.18) are dimensionless.

Note 2: The terms "-0.034" and "0.056" are assumed to have the units [ft].

Figure 1.6.2.3
Calculate DEPTH OF FLOW

(DF)

DF - DEPTH OF FLOW [ft]. Depth of flow for average annual erosion using a two-year period peak discharge flowing over the area.

STORM
LENGT - - -> DF <—— VEL

Short Name	Long Name	SI Unit	Source
DF	DEPTH OF FLOW	[ft]	1.6.2.3
LENGT	TOTAL LENGTH OF TAILINGS PILE	[ft]	1.6.1.1
STORM	MAX. 24-HR. RAINFALL	[mm d^{-1}]	Sampled
VEL	FLOW VELOCITY THROUGH GRASS	[ft s^{-1}]	1.6.2.2

$$DF = \frac{STORM * LENGT}{VEL * 2.633 * 10^{7}}$$

(equation supplied by SENES in a letter 1987-01-13, response #74; see Note 2)

Unit check:

$$\frac{[\mathrm{mm}\ d^{-1}] * [\mathrm{ft}]}{[\mathrm{ft}\ s^{-1}] * [\mathrm{mm}\ d^{-1}\ \mathrm{ft}^{-1}\ s]} = [\mathrm{ft}]$$

Note 1: Units of 2.633×10^{7} are [mm d^{-1} ft^{-1} s] as given in SENES letter (1987-01-13), response #74.

Note 2: LENGT is assumed to be equivalent to "L" in responses #74 and 76 of the SENES letter of 1987-01-13.

Figure 1.6.2.4
Calculate SPACING
HYDRAULIC RADIUS
(RS)

RS - SPACING HYDRAULIC RADIUS [ft].
Hydraulic radius for flow over partially vegetated tailings.

DF
SPACE ⟶ RS

Short Name	Long Name	SI Unit	Source
DF	DEPTH OF FLOW	[ft]	1.6.2.3
RS	SPACING HYDRAULIC RADIUS	[ft]	1.6.2.4
SPACE	AVERAGE GRASS SPACING	[ft]	1.6.2.1

RS = DF * SPACE / (2 * DF + SPACE) (page 3-128)

Unit check:
[ft] * [ft] / ([ft] + [ft]) = [ft]

DMID - MEAN SILT DIAMETER [ft].
The mean diameter of silt particles from the tailings.

Figure 1.6.2.5
Calculate MEAN SILT DIAMETER (DMID)

DM - - -> DMID

Short Name	Long Name	SI Unit	Source
DM	MEAN METRIC SILT DIAMETER	[mm]	Sampled
DMID	MEAN SILT DIAMETER	[ft]	1.6.2.5

$$DMID = DM / 308.4$$

(equation given in SENES letter 1987-01-13, response #71)

Unit check:

DMID $[mm] / [mm\ ft^{-1}] = [ft]$

Note 1: DM is not in SENES Vol. 3 but is sampled from constant (0.01) [mm] (SENES letter 1987-01-13, response #71).

Note 2: Units of 308.4 are $[mm\ ft^{-1}]$ (response #71).

VS - SETTLING VELOCITY [ft s^{-1}].
Settling velocity of silt- and clay-size particles.

Figure 1.6.2.6
Calculate SETTLING VELOCITY (VS)

$$\boxed{\begin{matrix} \text{NU} \\ \text{DMID} \end{matrix} \quad \text{- - ->} \quad \text{VS}}$$

Short Name	Long Name	SI Unit	Source
DMID	MEAN SILT DIAMETER	[ft]	1.6.2.5
NU	KINEMATIC VISCOSITY	[ft^2 s^{-1}]	Sampled
VS	SETTLING VELOCITY	[ft s^{-1}]	1.6.2.6

$$VS = \left(\frac{2}{9}\right) * (32.2) * \frac{(DMID)^2}{NU} * (2.65-1) \qquad \text{(eqn. 3.14.16)}$$

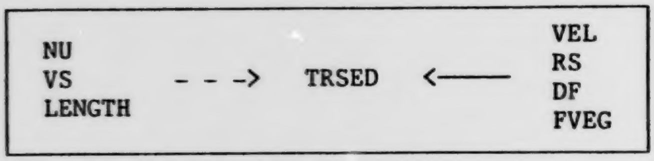
Unit check:

$$VS = \frac{[-]}{[-]} * [ft\ s^{-2}] * \frac{[ft]^2}{[ft^2\ s^{-1}]} * [-] = [ft\ s^{-1}]$$

Note: "2" and "9" are dimensionless from definitions in the Stokes' equation. Specific gravities "2.65" and "1" are dimensionless by definition. 32.2 is the gravitational constant in [ft s^{-2}].

Figure 1.6.2.7
Calculate FRACT.
TRAPPED SED.
(TRSED)

TRSED - FRACT. TRAPPED SED. [-].
Fraction of the suspended sediment trapped by vegetation.



Short Name	Long Name	SI Unit	Source
DF	DEPTH OF FLOW	[ft]	1.6.2.3
FVEG	FRACT. TAILINGS VEG.	[-]	1.6.1.7
LENGTH	LENGTH OF A SLOPE SEGMENT	[ft]	1.6.1.3
NU	KINEMATIC VISCOSITY	$[ft^2\ s^{-1}]$	Sampled
RS	SPACING HYDRAULIC RADIUS	[ft]	1.6.2.4
TRSED	FRACT. TRAPPED SED.	[-]	1.6.2.7
VEL	FLOW VELOCITY THROUGH GRASS	$[ft\ s^{-1}]$	1.6.2.2
VS	SETTLING VELOCITY	$[ft\ s^{-1}]$	1.6.2.6

$$TRSED = EXP\left\{(-1.05*10^{-3}) * \left[\frac{VEL*RS}{NU}\right]^{0.82} * \left[\frac{LENGTH * VS}{VEL * DF}\right]^{-0.91}\right\}$$

(eqn. 3.14.15;
modified 1987-01-27,
SENES letter)

Unit check:

$$[-] * \left[\frac{[ft\ s^{-1}] * [ft]}{[ft^2\ s^{-1}]}\right]^{0.82} * \left[\frac{[ft] * [ft\ s^{-1}]}{[ft\ s^{-1}] * [ft]}\right]^{-0.91} = [-]$$

Note 1: It is assumed that $\lambda \equiv LENGTH$ is the required distance in the equation for Tr_j, as described in SENES letters 1987-01-27 and 1987-01-03.

Note 2: The constants in eqn. (3.14.15) are assumed to be dimensionless (response #74).

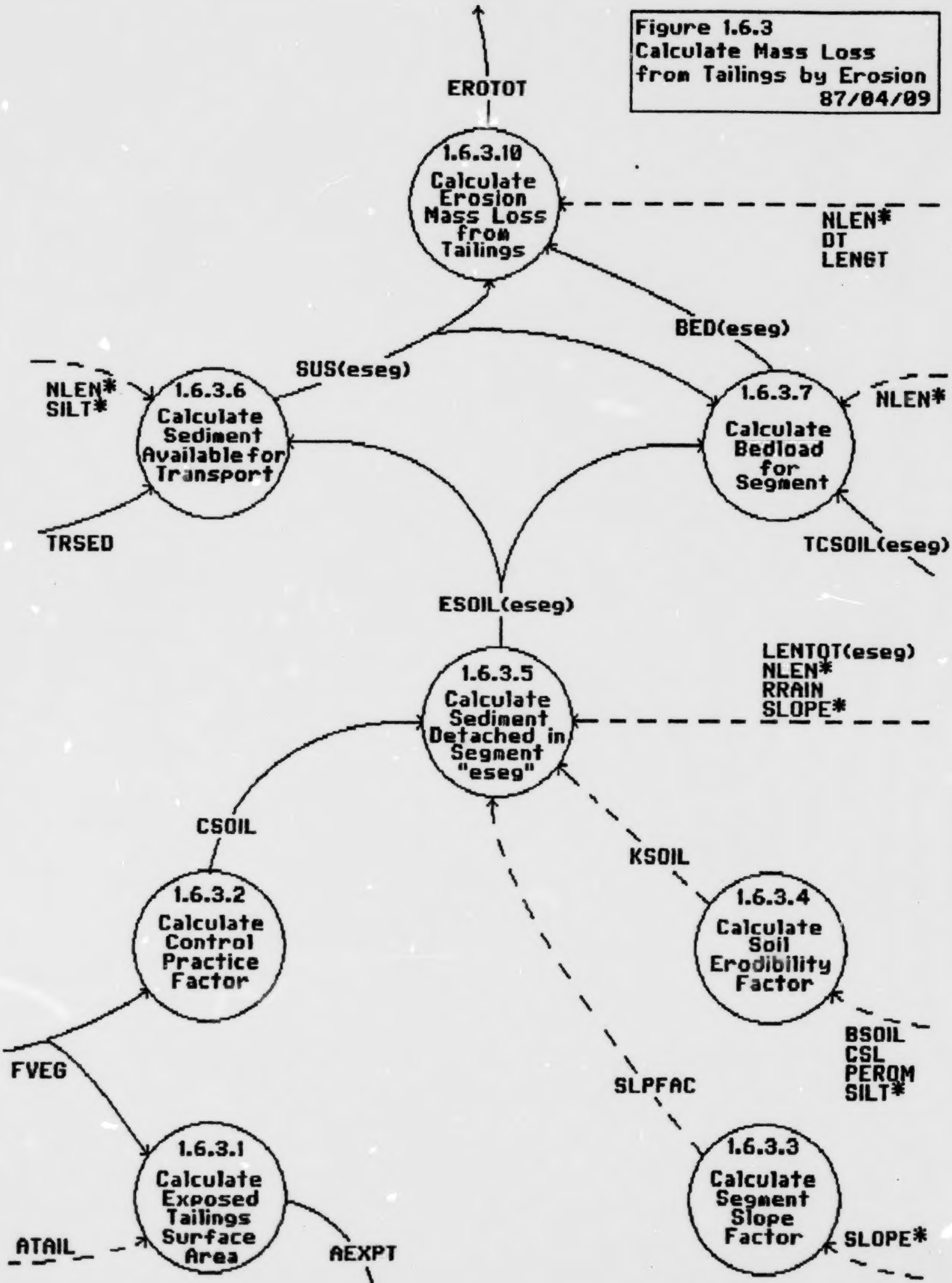


Figure 1.6.3
Calculate Mass Loss
from Tailings by Erosion
87/04/09

EROTOT
1.6.3.10
Calculate Erosion Mass Loss from Tailings
NLEN*
DT
LENGT
BED(eseg)
SUS(eseg)
NLEN*
SILT*
1.6.3.6
Calculate Sediment Available for Transport
TRSED
1.6.3.7
Calculate Bedload for Segment
NLEN*
TCSOIL(eseg)
ESOIL(eseg)
LENTOT(eseg)
NLEN*
RRAIN
SLOPE*
1.6.3.5
Calculate Sediment Detached in Segment "eseg"
CSOIL
KSOIL
1.6.3.2
Calculate Control Practice Factor
1.6.3.4
Calculate Soil Erodibility Factor
BSOIL
CSL
PEROM
SILT*
FVEG
SLPFAC
1.6.3.1
Calculate Exposed Tailings Surface Area
ATAIL
AEXPT
1.6.3.3
Calculate Segment Slope Factor
SLOPE*

Figure 1.6.3.1
Calculate EXPOSED
TAILINGS SURFACE AREA
(AEXPT)
and
Figure 1.6.3.2
Calculate CONTROL
PRACTICE FACTOR
(CSOIL)

AEXPT - EXPOSED TAILINGS SURFACE AREA [m^2].
Exposed surface area of the tailings, as a function of time.

CSOIL - CONTROL PRACTICE FACTOR [-].
Erosion control factor, treated here as exclusively a function of the amount of vegetation cover of the tailings.

$$\begin{tikzcd} \text{AEXPT} & \begin{array}{l}\text{ATAIL}\\ \text{FVEG}\end{array} \arrow[l] \\ \text{CSOIL} & \text{FVEG} \arrow[l] \end{tikzcd}$$

Short Name	Long Name	SI Unit	Source
AEXPT	EXPOSED TAILINGS SURFACE AREA	[m^2]	1.6.3.1
ATAIL	INITIAL EXPOSED TAILINGS SURFACE AREA	[m^2]	Sampled
CSOIL	CONTROL PRACTICE FACTOR	[-]	1.6.3.2
FVEG	FRACT. TAILINGS VEG.	[-]	1.6.1.7

$$\text{AEXPT} = (1.0 - \text{FVEG}) * \text{ATAIL}$$ (see Note 1)

If FVEG = 0
$$\text{CSOIL} = 1$$ (below eqn. 3.14.6)

If FVEG > 0
$$\text{CSOIL} = \text{EXP}\,[-0.109 - 0.056 * \text{FVEG}]$$ (eqn. 3.14.6; see Note 2)

Unit check: AEXPT $([-] - [-]) * [m^2] = [m^2]$

CSOIL $\text{EXP}\,([-] - [-] * [-]) = [-]$

Note 1: Inferred from the definition of FVEG (page 3-123) and confirmed by a letter from SENES (1986-10-15).

Note 2: -0.109 and 0.056 are assumed to be dimensionless.

Note 3: Inspection of the UTAP2 code shows some variance for the calculations of CSOIL. SYVAC3-UT2 has implemented the logic shown in Note 4 of DDD 1.6.1.7.

Figure 1.6.3.3
Calculate SEGMENT
SLOPE FACTOR
(SLPFAC)

SLPFAC - SEGMENT SLOPE FACTOR [-].
The slope factor in the universal soil loss equation (for any segment).

SLOPE - - -> SLPFAC

Short Name	Long Name	SI Unit	Source
SLOPE	TAILINGS SLOPE	[-]	Sampled
SLPFAC	SEGMENT SLOPE FACTOR	[-]	1.6.3.3

$$\mathrm{SLPFAC} = \left[0.43 + 0.30 * \mathrm{SLOPE} + 0.043 * \mathrm{SLOPE}^2\right] / 6.613$$

(eqn. 3.14.3; revised in a letter from senes 1987-01-13, response #70; see Note 2)

Unit check:

$$\mathrm{SLPFAC} \quad \left[[-] + [-] * [-] + [-] * [-]^2\right] / [-] = [-]$$

Note 1: The numbers "0.43", "0.30", "0.043" and "6.613" are assumed to be dimensionless.

Note 2: Inspection of the UTAP2 code shows that the equation used is

$$\mathrm{SLPFAC} = [0.43 + 0.30 * \mathrm{SLOPE} + (0.43 * \mathrm{SPRIME})^2] / 6.613$$

where $\mathrm{SPRIME} = \mathrm{SIN}\left[\mathrm{ATAN}\left(\frac{\mathrm{SLOPE}}{100}\right)\right]$

This equation has been implemented in SYVAC3-UT2. (BWG, 87-04-10)

KSOIL - SOIL ERODIBILITY FACTOR [-].
The factor in the universal soil loss equation that relates erosion to soil type.

Figure 1.6.3.4
Calculate SOIL ERODIBILITY FACTOR (KSOIL)

PEROM
CSL
BSOIL - - -> KSOIL
MSOIL

SILT - - -> MSOIL

Short Name	Long Name	SI Unit	Source
BSOIL	SOIL STRUCT. CODE	[-]	Sampled
CSL	SOIL PERM. CLASS	[-]	Sampled
KSOIL	SOIL ERODIBILITY FACTOR	[-]	1.6.3.4
MSOIL	SILT FACTOR	[-]	(1.6.3.4)
PEROM	PERCENT ORGANIC	[-]	Sampled
SILT	SILT CONTENT OF TAILINGS SURFACE	[-]	Sampled

$$MSOIL = SILT * 100 \qquad \text{(below eqn. 3.14.4)}$$

$$KSOIL = [2.1 * MSOIL^{1.14} * 10^{-4} * (12-PEROM) + 3.25 * (BSOIL-2) + 2.5 * (CSL-3)] / 100 \qquad \text{(eqn. 3.14.4)}$$

Unit check:

$$MSOIL\ \ [-] * [-] = [-]$$

$$KSOIL\ \ ([-]*[-]*[-]*([-]-[-])+[-]*([-]-[-])+[-]*([-]-[-])\ /\ [-] = [-]$$

Note 1: Although noted as Kj on SENES Vol. 3 pg. 3-120, KSOIL is not segment dependent in the current model.

Note 2: The equation for MSOIL includes the assumption (SENES Vol. 3 pg. 3-120) that the percentage clay in the soil is zero.

Note 3: All numerical constants were assumed dimensionless.

Note 4: The value of CSL was provided in letters from SENES (1986-12-02 and 1987-01-13).

Figure 1.6.3.5
Calculate SEDIMENT DETACHED IN SEGMENT "eseg" (ESOIL(eseg))

ESOIL(eseg) - SEDIMENT DETACHED IN SEGMENT "eseg" [lb ft^{-1} a^{-1}]. The quantity of material eroded annually from the tailings pile in segment "eseg", as calculated from the Universal Soil Loss Equation.

```
NLEN
RRAIN
KSOIL
SLPFAC          - - ->  ESOIL(eseg) <-----  CSOIL
LENTOT(eseg)
MSLP

SLOPE           - - ->  MSLP
```

Short Name	Long Name	SI Unit	Source
CSOIL	CONTROL PRACTICE FACTOR	[-]	1.6.3.2
ESOIL(eseg)	SEDIMENT DETACHED IN SEGMENT "eseg"	[lb ft^{-1} a^{-1}]	1.6.3.5
KSOIL	SOIL ERODIBILITY FACTOR	[-]	1.6.3.4
LENTOT(eseg)	TOTAL LENGTH TO END SEGMENT "eseg"	[ft]	1.6.1.10
MSLP	USLE EXPONENT	[-]	(1.6.3.5)
NLEN	NUMBER OF SLOPE SEGMENTS	[-]	1.1.6.2
RRAIN	RAINFALL EROS. FACTOR	[100(ft tons acre^{-1})(in hr)]	Sampled
SLOPE	TAILINGS SLOPE	[-]	Sampled
SLPFAC	SEGMENT SLOPE FACTOR	[-]	1.6.3.3

If $\mathrm{SLOPE} \leq 3.0$ $\quad \mathrm{MSLP} = 0.3$

If $3 < \mathrm{SLOPE} < 5$ $\quad \mathrm{MSLP} = 0.4$ (below eqn. 3.14.3; see Note 2)

If $5 \leq \mathrm{SLOPE}$ $\quad \mathrm{MSLP} = 0.5$

for $\mathrm{NLEN} \geq \mathrm{eseg} \geq 1$,

$$\mathrm{ESOIL(eseg)} = \left\{ [0.0459 * \mathrm{RRAIN} * \mathrm{KSOIL} * \mathrm{CSOIL} * \mathrm{SLPFAC} * \frac{\left[(\mathrm{LENTOT(eseg)})^{(\mathrm{MSLP}+1)} - (\mathrm{LENTOT(eseg-1)})^{(\mathrm{MSLP}+1)}\right]}{72.6^{\mathrm{MSLP}}} \right\}$$

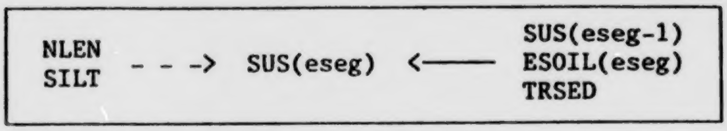
(eqn. 3.14.2; see Note 1)

Unit check: ESOIL

$$\frac{[\mathrm{lb\ ft}^{-2}\ \mathrm{a}^{-1}\ (\text{units of RRAIN})^{-1}]*[\text{units of RRAIN}]*[-]*[-]*[-]*[\mathrm{ft}]^{\mathrm{MSLP}+1}}{[\mathrm{ft}]^{\mathrm{MSLP}}}$$

$$= [\mathrm{lb\ ft}^{-1}\ \mathrm{a}^{-1}]$$

Note 0: Equation 3.14.2 was modified in a letter from SENES (1987-01-13), response #76.
Note 1: Assume that LENTOT(0) = 0.
Note 2: Values for MSLP modified in a letter from SENES (1987-01-27).
Note 3: To obtain a consistent unit check it has been necessary to assume units of [ft] for the constant "72.6" and [lb ft^{-2} a^{-1} (units of RRAIN)$^{-1}$] for 0.0459.
Note 4: Use of LENTOT here confirmed by SENES letter (1987-01-13).



Short Name	Long Name	SI Unit	Source
ESOIL(eseg)	SEDIMENT DETACHED IN SEGMENT "eseg"	[lb ft^{-1} a^{-1}]	1.6.3.5
NLEN	NUMBER OF SLOPE SEGMENTS	[-]	1.6.1.2
SILT	SILT CONTENT OF TAILINGS SURFACE	[-]	Sampled
SUS(eseg)	SEDIMENT AVAILABLE FOR TRANSPORT	[lb ft^{-1} a^{-1}]	1.6.3.6
TRSED	FRACT. TRAPPED SED.	[-]	1.6.2.7

For eseg=1 to NLEN
from the finite difference equation

$$\text{SUS(eseg)} = \text{SUS(eseg-1)} + \text{ESOIL(eseg)} * \frac{\text{SILT}}{100} * \text{(1-TRSED)}$$

(eqn. 3.14.20 as
modified in SENES
letter 1987-01-27;
see Note 5)

Unit check:

$$[\text{lb ft}^{-1}\ \text{a}^{-1}] + [\text{lb ft}^{-1}\ \text{a}^{-1}] * \frac{[-]}{[-]} * ([-] - [-]) = [\text{lb ft}^{-1}\ \text{a}^{-1}]$$

Note 1: If eseg=1, SUS(eseg-1)≡0.

Note 2: "100" is dimensionless by definition.

Note 3: "1" is assumed dimensionless.

Note 4: It is not clear what the form is of the SENES equations, but this should be a useable form (see also SENES letter 1987-02-03).

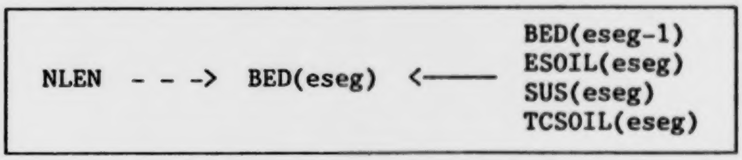
Note 5: Inspection of the UTAP2 code shows that the equation for SUS is

$$\text{SUS(eseg)} = \left\{\text{SUS(eseg-1)} + \text{ESOIL(eseg)} + \frac{\text{SILT}}{100}\right\} * \text{(1-TRSED)}$$

This revision has been implemented in SYVAC3-UT2. (BWG, 87-04-10)

Figure 1.6.3.7
Calculate BEDLOAD
FOR SEGMENT
(BED(eseg))

BED(eseg) - BEDLOAD FOR SEGMENT [lb ft^{-1} a^{-1}]. The bedload contribution to erosion for segment "eseg" of the tailings pile.



Short Name	Long Name	SI Unit	Source
BED(eseg)	BEDLOAD FOR SEGMENT	[lb ft^{-1} a^{-1}]	1.6.3.7
ESOIL(eseg)	SEDIMENT DETACHED IN SEGMENT "eseg"	[lb ft^{-1} a^{-1}]	1.6.3.5
NLEN	NUMBER OF SLOPE SEGMENTS	[-]	1.6.1.2
SUS(eseg)	SEDIMENT AVAILABLE FOR TRANSPORT	[lb ft^{-1} a^{-1}]	1.6.3.6
TCSOIL(eseg)	BEDLOAD TRANSPORT CAPACITY	[lb ft^{-1} a^{-1}]	1.6.1.11

for eseg=1 to NLEN

(i) BED(eseg) = BED(eseg-1) + ESOIL(eseg) - SUS(eseg)

(eqn. below eqn. 3.14.20 as modified in SENES letter 1987-01-27; see Note 3)

(ii) BED(eseg) = TCSOIL(eseg)

If BED(eseg) > TCSOIL(eseg)

Unit check: BED:

(i) [lb ft^{-1} a^{-1}] + [lb ft^{-1} a^{-1}] - [lb ft^{-1} a^{-1}] = [lb ft^{-1} a^{-1}]

(ii) [lb ft^{-1} a^{-1}] = [lb ft^{-1} a^{-1}]

Note 1: If eseg=1, BED(eseg-1)≡0.

Note 2: It is not clear what the form is of the SENES equations, but this should be a useable form (see also SENES letter 1987-02-03).

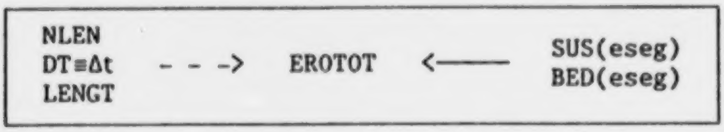
Note 3: Inspection of the UTAP2 code shows that the equation used for BED in (i) was:

$$\text{BED(eseg)} = \text{BED(eseg-1)} + \text{ESOIL(eseg)} * \left(1 - \left(\frac{\text{SILT}}{100}\right)\right.$$

This revision has been implemented in SYVAC3-UT2. (BWG, 87-04-10)

Figure 1.6.3.10
Calculate EROSION MASS
LOSS FROM TAILINGS
(EROTOT)

EROTOT - EROSION MASS LOSS FROM TAILINGS [kg].
The total sediment mass leaving the tailings pile in the time interval Δt.



Short Name	Long Name	SI Unit	Source
BED(eseg)	TOTAL BEDLOAD	[lb ft^{-1} a^{-1}]	1.6.3.7
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
EROTOT	EROSION MASS LOSS FROM TAILINGS	[kg]	1.6.3.10
LENGT	TOTAL LENGTH OF TAILINGS PILE	[ft]	1.6.1.1
NLEN	NUMBER OF SLOPE SEGMENTS	[-]	1.1.6.2
SUS(eseg)	TOTAL SUSPENDED SEDIMENT	[lb ft^{-1} a^{-1}]	1.6.3.6

$$\text{EROTOT} = \frac{\text{LENGT} * \text{NLEN} * (\text{SUS(NLEN)} + \text{BED(NLEN)}) * \text{DT}}{2.2}$$

(eqn. 3.14.21; see Note 3)

Unit check:

$$\frac{[\text{ft}] * [-] * ([\text{lb ft}^{-1}\ \text{a}^{-1}] + [\text{lb ft}^{-1}\ \text{a}^{-1}]) * [\text{a}]}{[\text{lb kg}^{-1}]} = [\text{kg}]$$

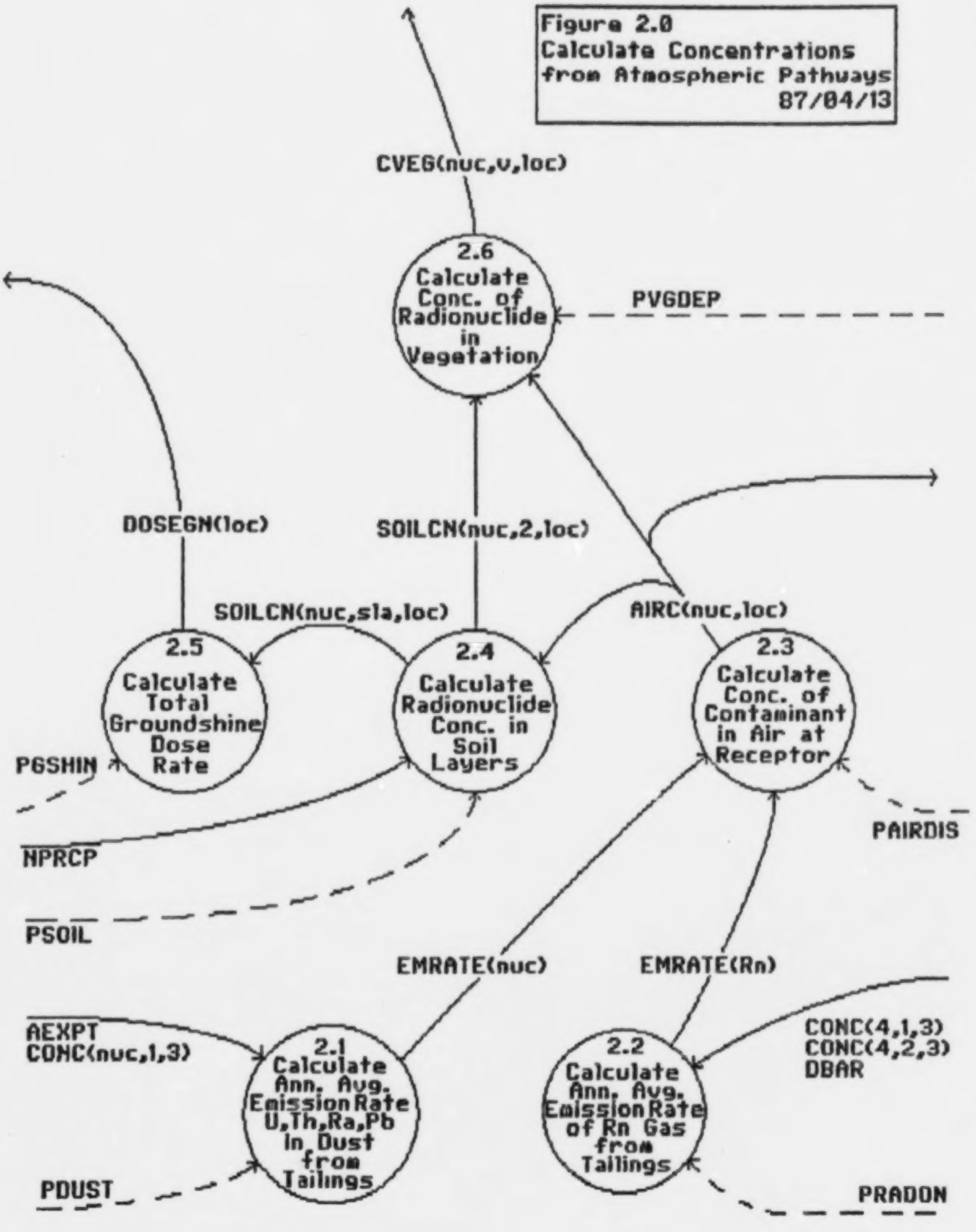
Note 1: This assumes the factor 2.2 in the denominator is the conversion factor 2.2 [lb kg^{-1}].

Note 2: The use of "LENGT" here was confirmed by a letter from SENES (1987-01-13), response #76.

Note 3: Inspection of the UTAP2 code shows that the equation for EROTOT does not include multiplication by NLEN in the numerator. It has been accordingly removed from SYVAC3-UT2. (BWG, 87-04-10)

Note 4: The UTAP2 code also includes a variable called DTAIL which appears to be the depth of the depleted tailings (through erosion). DTAIL is zero at t=-Δt, and calculated as follows:
$\text{DTAIL}(t) = \text{DTAIL}(t-\Delta t) + 10^3 * \text{EROTOT} / (\text{RHOTAL} * \text{ATAIL})$.
It is not clear, however, whether this variable is used elsewhere within UTAP2. It is not implemented in SYVAC3-UT2. (BWG, 87-04-10)

Figure 2.0
Calculate Concentrations
from Atmospheric Pathways
87/04/13


CVEG(nuc,v,loc)
2.6
Calculate
Conc. of
Radionuclide
in
Vegetation
PVGDEP
DOSEGN(loc)
SOILCN(nuc,2,loc)
SOILCN(nuc,sla,loc)
AIRC(nuc,loc)
2.5
Calculate
Total
Groundshine
Dose
Rate
2.4
Calculate
Radionuclide
Conc. in
Soil
Layers
2.3
Calculate
Conc. of
Contaminant
in Air at
Receptor
PGSHIN
NPRCP
PAIRDIS
PSOIL
EMRATE(nuc)
EMRATE(Rn)
AEXPT
CONC(nuc,1,3)
2.1
Calculate
Ann. Avg.
Emission Rate
U,Th,Ra,Pb
In Dust
from
Tailings
2.2
Calculate
Ann. Avg.
Emission Rate
of Rn Gas
from
Tailings
CONC(4,1,3)
CONC(4,2,3)
DBAR
PDUST
PRADON

Note: nuc=U, Th, Pb and Ra for all variables except AIRC. For AIRC nuc=U, Th, Pb, Ra and Rn.

EMRATE(nuc) - ANN. AVG. EMISSION RATE OF RADIONUCLIDE IN DUST FROM TAILINGS [Bq s^{-1}]. Annual average emission rate of radionuclide (nuc=nat-U, tot-Th, Ra-226, Pb-210) in dust from the tailings surface as a function of time.

Figure 2.1
Calculate ANN. AVG. EMISSION RATE OF RADIONUCLIDE IN DUST FROM TAILINGS (EMRATE(nuc), nuc=nat-U, tot-Th, Ra-226, Pb-210)
(Page 1 of 2)

NSUBW - - -> EMRATE(nuc) <—— Q(nuc)

SILT, FWINDT, FPREC, RHOTAL - - -> Q(nuc) <—— CONC(nuc,1,3), AEXPT

FWIND(dir,st,vel,yr) - - -> FWINDT

Short Name	Long Name	SI Unit	Source
AEXPT	EXPOSED TAILING SURFACE AREA	[m^2]	1.6.3.1
CONC(nuc,1,3)	CONC. SOLID RADIONUCLIDE IN LAYER 1	[Bq m^{-3}]	1.2.3, 1.3.2.5B, 1.4.1.4, 1.5.1.3
EMRATE(nuc)	ANN. AVG. EMISSION RATE OF RADINOUCLIDE IN DUST FROM TAILINGS	[Bq s^{-1}]	2.1
FPREC	ANNUAL DAYS WITH SIG. PRECIP.	[d a^{-1}]	Sampled
FWIND(dir,st,vel,yr)	FRACTION OF WIND TYPE	[-]	Sampled
FWINDT	FRACTION OF TIME WITH HIGH WIND SPEEDS	[-]	(2.1)
NSUBW	WINTER MONTHS PER YEAR	[months a^{-1}]	Sampled
Q(nuc)	EMISSION RATE OF RADIONUCLIDE IN DUST FROM TAILINGS SURFACE	[Bq s^{-1}]	(2.1)
RHOTAL	TAILINGS BULK DENSITY	[g m^{-3}]	Sampled
SILT	SILT CONTENT OF TAILINGS SURFACE	[-]	Sampled

$$\text{FWINDT} = \sum_{dir=1}^{16} \sum_{st=1}^{6} \sum_{vel=4}^{6} \text{FWIND}(dir,st,vel,yr)$$

(eqn. supplied by SENES, letter 1986-11-04)

$$\text{Q(nuc)} = \frac{2.2 * 10^{-6} * \text{SILT} * (365-\text{FPREC}) * \text{FWINDT} * \text{CONC}(nuc,1,3) * \text{AEXPT}}{1.5 * 235 * 0.15 * \text{RHOTAL}}$$

nuc = nat-U,tot-Th,Ra-226,Pb-210)
(eqn. 4.7)

$$\text{EMRATE(nuc)} = \text{Q(nuc)} * \frac{(12 - \text{NSUBW})}{12} \qquad \text{(eqn. 4.8)}$$

Figure 2.1
Calculate ANN. AVG.
EMISSION RATE OF
RADIONUCLIDE IN DUST
FROM TAILINGS
(EMRATE(nuc), nuc=nat-U,
tot-Th, Ra-226, Pb-210)
(Page 2 of 2)

Unit check:

FWINDT: $\Sigma\,[-] = [-]$

Q(nuc): $$[\mathrm{g\ m^{-2}\ s^{-1}}] * \frac{[-] * [\mathrm{d\ a^{-1}}] * [-] * [\mathrm{Bq\ m^{-3}}] * [\mathrm{m^2}]}{[-] * [\mathrm{d\ a^{-1}}] * [-] * [\mathrm{g\ m^{-3}}]} = [\mathrm{Bq\ s^{-1}}]$$
(see Note)

EMRATE(nuc): $[\mathrm{Bq\ s^{-1}}] * [\mathrm{months\ a^{-1}}] / [\mathrm{months\ a^{-1}}] = [\mathrm{Bq\ s^{-1}}]$
(see Note)

Note: The constant 2.2×10^{-6} has units of $[\mathrm{g\ m^{-2}\ s^{-1}}]$. 1.5 and 0.15 are assumed dimensionless. 365 and 235 are assumed to have units of $[\mathrm{days\ a^{-1}}]$. The value 12 in eqn. (4.8) is assumed to be $[\mathrm{months\ a^{-1}}]$.

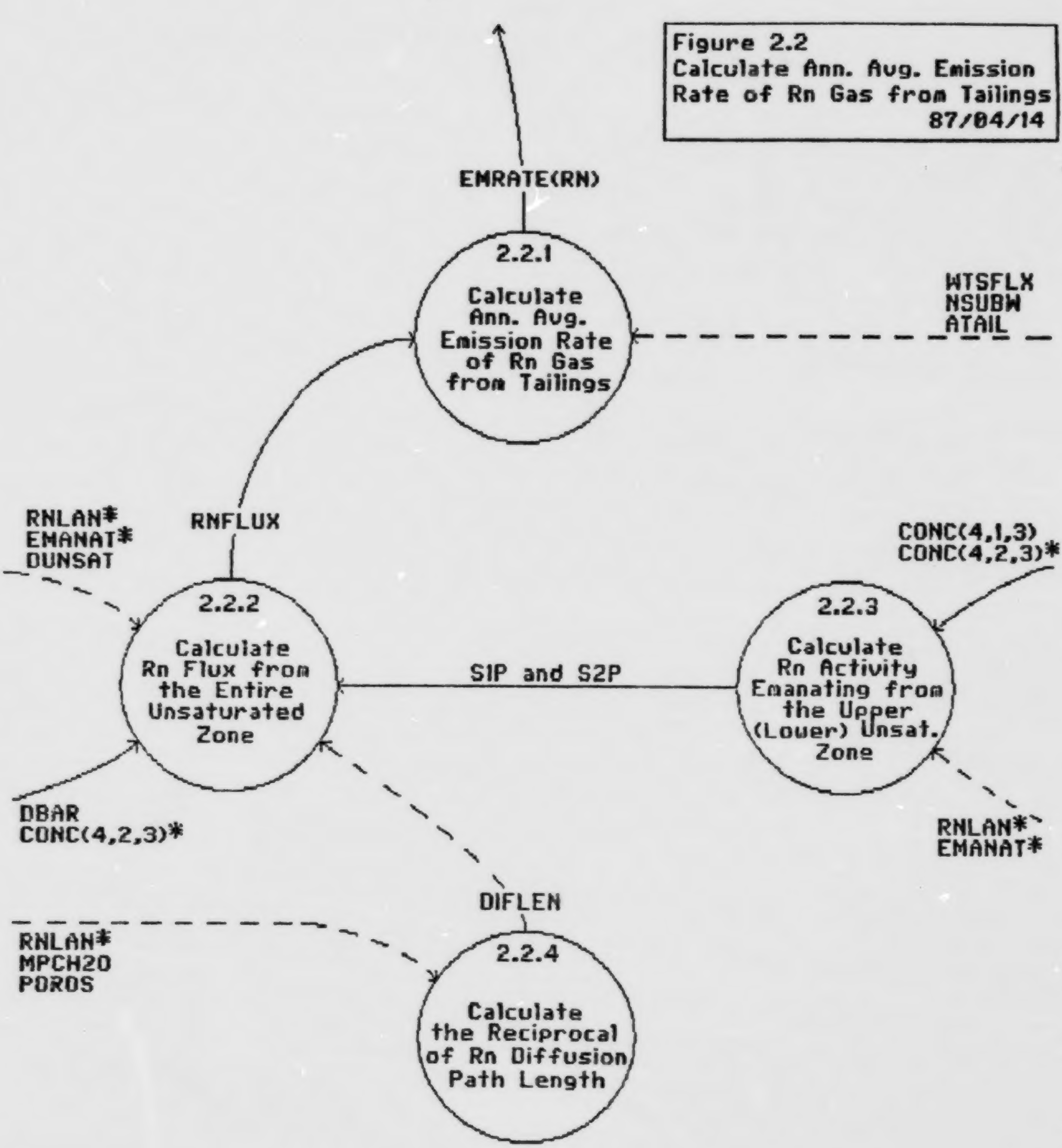


Figure 2.2
Calculate Ann. Avg. Emission
Rate of Rn Gas from Tailings
87/04/14

EMRATE(RN)
2.2.1
Calculate Ann. Avg. Emission Rate of Rn Gas from Tailings
WTSFLX
NSUBW
ATAIL
RNFLUX
RNLAN*
EMANAT*
DUNSAT
2.2.2
Calculate Rn Flux from the Entire Unsaturated Zone
S1P and S2P
CONC(4,1,3)
CONC(4,2,3)*
2.2.3
Calculate Rn Activity Emanating from the Upper (Lower) Unsat. Zone
DBAR
CONC(4,2,3)*
RNLAN*
EMANAT*
DIFLEN
RNLAN*
MPCH2O
POROS
2.2.4
Calculate the Reciprocal of Rn Diffusion Path Length

Figure 2.2.1
Calculate ANN. AVG. EMISSION RATE OF RN GAS FROM TAILINGS (EMRATE(RN))

EMRATE(RN) - ANN. AVG. EMISSION RATE OF RN GAS FROM TAILINGS [Bq s^{-1}]. Annual average emission rate of Rn-222 gas from the tailings unsaturated zone (upper and lower layers) as a function of time.

ATAIL - - -> EMRATE(RN) <—— RNFXAV

NSUBW
WTSFLX - - -> RNFXAV <—— RNFLUX

Short Name	Long Name	SI Unit	Source
ATAIL	INITIAL EXPOSED TAILINGS SURFACE AREA	[m^2]	Sampled
EMRATE(RN)	ANN. AVG. EMISSION RATE OF RN GAS FROM TAILINGS	[Bq s^{-1}]	2.2.1
NSUBW	WINTER MONTHS PER YEAR	[months a^{-1}]	Sampled
RNFLUX	RN FLUX FROM THE ENTIRE UNSATURATED ZONE	[Bq m^{-2} s^{-1}]	2.2.2
RNFXAV	ANN. AVG. RN FLUX FROM THE ENTIRE UNSATURATED ZONE	[Bq m^{-2} s^{-1}]	(2.2.1)
WTSFLX	RATIO OF RN FLUXES FROM FROZEN AND UNFROZEN TAILINGS	[-]	Sampled

$$RNFXAV = RNFLUX * (NSUBW * WTSFLX + (12 - NSUBW)) / 12$$

$$EMRATE(RN) = RNFXAV * ATAIL \qquad \text{(eqn. 4.5)}$$

Unit check:

RNFXAV: $[\text{Bq m}^{-2}\ \text{s}^{-1}] * ([\text{months a}^{-1}] * [-] + ([\text{months a}^{-1}])) / [\text{months a}^{-1}] = [\text{Bq m}^{-2}\ \text{s}^{-1}]$

EMRATE: $[\text{Bq m}^{-2}\ \text{s}^{-1}] * [\text{m}^2] = [\text{Bq s}^{-1}]$

Note: The constants "12" used in the equation for RNFXAV are assumed to have units [months a^{-1}].

Figure 2.2.2
Calculate RN FLUX FROM THE ENTIRE UNSATURATED ZONE (RNFLUX)

RNFLUX - RN FLUX FROM THE ENTIRE UNSATURATED ZONE [Bq m^{-2} s^{-1}]. Rn-222 flux from the upper ($BaSO_4$ depleted) and lower ($BaSO_4$ enriched) layers of the unsaturated zone, as a function of time.

DIFLEN
DUNSAT - - -> RNFLUX <—— DBAR
S1P (and S2P)

Short Name	Long Name	SI Unit	Source
DBAR	THICKNESS $BASO_4$ DEPLETED LAYER	[m]	1.4.2.4
DIFLEN	RECIPROCAL OF RN DIFFUSION PATH LENGTH	[m^{-1}]	2.2.4
DUNSAT	DEPTH OF UNSAT. ZONE	[m]	Sampled
RNFLUX	RN FLUX FROM THE ENTIRE UNSATURATED ZONE	[Bq m^{-2} s^{-1}]	2.2.2
S1P(and S2P)	RN ACTIVITY EMANATING FROM THE UPPER (LOWER) UNSAT. ZONE	[Bq m^{-3} s^{-1}]	2.2.3

(a) If DBAR $\geq$ (DUNSAT - 1.E-3)

$$\text{RNFLUX} = \frac{\text{S1P}}{\text{DIFLEN}} * \text{TANH (DIFLEN * DUNSAT)}$$

(eqn. 4.2; see Note 1)

(b) If DBAR < (DUNSAT - 1.E-3)

$$\text{RNFLUX} = \frac{-\text{S1P}}{\text{DIFLEN}} + \frac{1}{\text{DIFLEN * COSH (DIFLEN * DBAR)}} *$$

$$\frac{\text{[1 + COTH(DIFLEN * (DUNSAT-DBAR)] * S1P * EXP(DIFLEN*DBAR) - S1P + S2P}}{\text{TANH(DIFLEN*DBAR) + COTH(DIFLEN * (DUNSAT-DBAR))}}$$

(eqn. 4.4; see Note 2)

Unit check:

$$\text{(a)}\quad \left(\frac{[\text{Bq m}^{-3}\ \text{s}^{-1}]}{[\text{s}^{-1}]}\right) * \left(\frac{[\text{s}^{-1}] * [\text{s}^{-1}]}{[\text{m}^{-1}]^{2}}\right)^{0.5} * \text{TANH}\ ([\text{m}^{-1}] * [\text{m}]) = [\text{Bq m}^{-2}\ \text{s}^{-1}]$$

$$\text{(b)}\quad \frac{[\text{Bq m}^{-3}\ \text{s}^{-1}]}{[\text{m}^{-1}]} + \frac{1}{[\text{m}^{-1}] * [-]}\left(([-] + [-] * [\text{Bq m}^{-3}\ \text{s}^{-1}] * [-]\right.$$

$$\left. - [\text{Bq m}^{-3}\ \text{s}^{-1}] + [\text{Bq m}^{-3}\ \text{s}^{-1}]\right) = [\text{Bq m}^{-2}\ \text{s}^{-1}]$$

Note 1: The value of x_1 is assumed equal to DUNSAT from the text above eqn. 4.2. S1P and DIFLEN have been used to modify (simplify) the equation. x_2 = (DUNSAT - DBAR)

Note 2: Equation 4.4 has been modified from that used in SENES Vol. 3 by use of S1P and S2P rather than S1 and S2.

Note 3: CONC(4,1,3) is in [Bq m^{-3}] and the tailings density is not required in eqn. (4.2).

S1P (and S2P) - RN ACTIVITY EMANATING FROM THE UPPER (LOWER) UNSAT. ZONE [Bq m^{-3} s^{-1}]. Proportional to the rate of emission of Rn-222 per unit area from the upper $BaSO_4$ depleted (and lower $BaSO_4$ enriched) layer of the unsaturated zone.

Figure 2.2.3
Calculate RN ACTIVITY EMANATING FROM THE UPPER (LOWER) UNSAT. ZONE (S1P (and S2P))

RNLAN
EMANAT - - -> S1P (and S2P) <—— CONC(4,1,3)
CONC(4,2,3)

Short Name	Long Name	SI Unit	Source
CONC(4,1,3)	CONC. SOLID RA IN LAYER 1	[Bq m^{-3}]	1.4.1.4
CONC(4,2,3)	CONC. SOLID RA IN LAYER 2	[Bq m^{-3}]	1.4.3.4
EMANAT	EMANATION COEFFICIENT	[-]	Sampled
RNLAN	RN-222 DECAY CONSTANT	[a^{-1}]	Sampled

S1P = CONC(4,1,3) * RNLAN * EMANAT

S2P = CONC(4,2,3) * RNLAN * EMANAT

(eqn. on pg. 4-2; see Notes)

Unit check:
S1P/S2P: [Bq m^{-3}] * [s^{-1}] * [-] = [Bq m^{-3} s^{-1}]

Note 1: The above equations have been modified from those used in SENES Vol. 3, pg. 4-2. The factor D_i has been incorporated in S1P ≡ S1 * D1 and S2P ≡ S2 * D2 since it cancels with the factor D_i in eqn. (4.4), the only place S1 and S2 are used.

Note 2: The tailings density is not needed in equation (4.2) as CONC(4,1,3) and CONC(4,2,3) are in [Bq m^{-3}].

Figure 2.2.4
Calculate RECIPROCAL OF RN DIFFUSION PATH LENGTH (DIFLEN)

DIFLEN - RECIPROCAL OF RN DIFFUSION PATH LENGTH $[m^{-1}]$. Reciprocal of the Rn-222 diffusion path length.

RNLAN
EBKDFC - - -> DIFLEN
POROS

POROS
MPCH2O - - -> EBKDFC

Short Name	Long Name	SI Unit	Source
DIFLEN	RECIPROCAL OF RN DIFFUSION PATH LENGTH	$[m^{-1}]$	2.2.4
EBKDFC	EFFECTIVE BULK DIFFUSION COEFFICIENT	$[m^2\ s^{-1}]$	(2.2.4)
MPCH20	PERCENT MOISTURE CONTENT OF TAILINGS	[-]	Sampled
POROS	TAILINGS POROSITY	[-]	Sampled
RNLAN	RN-222 DECAY CONSTANT	$[a^{-1}]$	Sampled

$$\text{EBKDFC} = 0.106 \times 10^{-4} * \text{POROS} * \text{EXP}\ (-0.261 * \text{MPCH2O}) \qquad \text{(eqn. 4.3)}$$

$$\text{DIFLEN} = (\text{RNLAN} * \text{POROS} / \text{EBKDFC})^{1/2} \qquad \text{(eqn. near 4.1)}$$

Unit check:

not possible for EBKDFC, since the units of the constants are not given

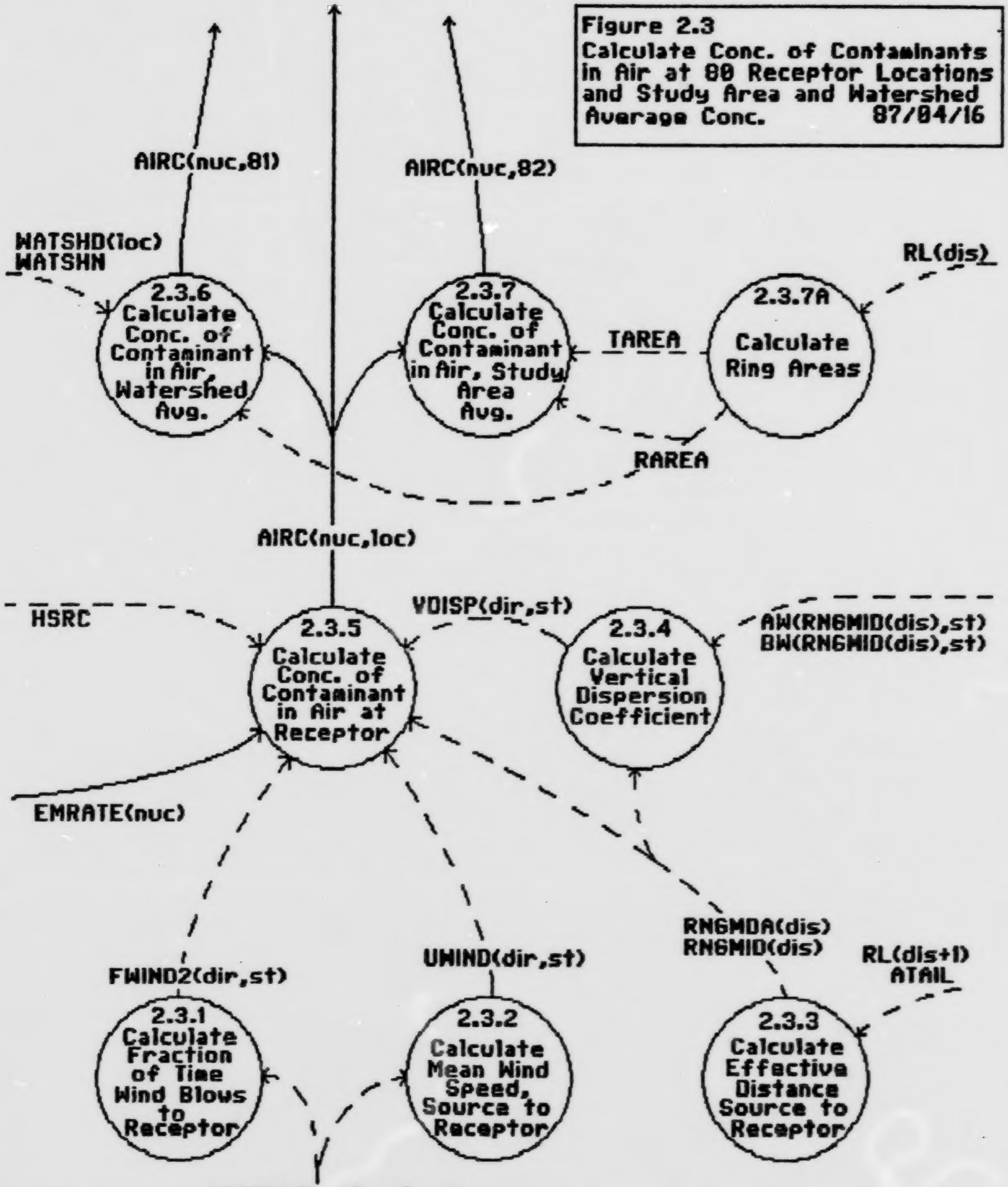
$$\text{DIFLEN:} \quad \left([s^{-1}] * [-] / [m^2\ s^{-1}]\right)^{1/2} = [m^{-1}]$$

Note 1: Combining the above,
$\text{DIFLEN} = \{\text{RNLAN} / [0.106 \times 10^{-4} * \text{EXP}\ (-0.261 * \text{MPCH2O})]\}^{1/2}$
which does not depend on POROS. This latter equation should not be used; see SENES Vol. 3, pg. 4-4.

Note 2: The constants used in EBKDFC have unknown dimensions.

Note 3: Assumes $\varepsilon_i \equiv \varepsilon \equiv$ POROS.

Figure 2.3
Calculate Conc. of Contaminants in Air at 80 Receptor Locations and Study Area and Watershed Average Conc. 87/04/16



AIRC(nuc,81)
AIRC(nuc,82)
WATSHD(loc)
WATSHN
RL(dis)
2.3.6 Calculate Conc. of Contaminant in Air, Watershed Avg.
2.3.7 Calculate Conc. of Contaminant in Air, Study Area Avg.
2.3.7A Calculate Ring Areas
TAREA
RAREA
AIRC(nuc,loc)
HSRC
VDISP(dir,st)
AW(RNGMID(dis),st)
BW(RNGMID(dis),st)
2.3.5 Calculate Conc. of Contaminant in Air at Receptor
2.3.4 Calculate Vertical Dispersion Coefficient
EMRATE(nuc)
RNGMDA(dis)
RNGMID(dis)
FWIND2(dir,st)
UWIND(dir,st)
RL(dis+1)
ATAIL
2.3.1 Calculate Fraction of Time Wind Blows to Receptor
2.3.2 Calculate Mean Wind Speed, Source to Receptor
2.3.3 Calculate Effective Distance Source to Receptor
FWIND(dir,st,vel,yr)

Note: in this DFD, nuc=U,Th,Pb,Ra and Rn; loc = 1 to 80; and dir, dis, st, yr and vel are wind-data indices.

FWIND2(dir,st) - FRACTION OF TIME WIND BLOWS TO RECEPTOR [-]. Fraction of the time the wind blows from the tailings source to the receptor (a man or vegetation) in a particular direction "dir" with a particular atmospheric stability "st".

UWIND(dir,st) - MEAN WIND SPEED, SOURCE TO RECEPTOR [m s^{-1}]. Mean annual wind speed in a particular direction "dir", and of a particular stability class "st".

Figure 2.3.1
Calculate FRACTION OF TIME WIND BLOWS TO RECEPTOR (FWIND2(dir,st))
and
Figure 2.3.2
Calculate MEAN WIND SPEED, SOURCE TO RECEPTOR (UWIND(dir,st))

FWIND(dir,st,vel,yr) - - -> FWIND2(dir,st)

FWIND(dir,st,vel,yr) - - -> UWIND(dir,st)

Short Name	Long Name	SI Unit	Source
FWIND(dir,st,vel,yr)	FRACTION OF WIND TYPE	[-]	Sampled
FWIND2(dir,st)	FRACTION OF TIME WIND BLOWS TO RECEPTOR	[-]	2.3.1
UWIND(dir,st)	MEAN WIND SPEED, SOURCE TO RECEPTOR	[m s^{-1}]	2.3.2

$$\text{FWIND2(dir,st)} = \sum_{v=1}^{6} \text{FWIND(dir,st,vel,yr)}$$

$$\begin{aligned}\text{UWIND(dir,st)} = \; & [1.50 \times \text{FWIND(dir,st,1,yr)} + \\ & 2.46 \times \text{FWIND(dir,st,[illegible],yr)} + \\ & 4.47 \times \text{FWIND(dir,st,3,yr)} + \\ & 6.93 \times \text{FWIND(dir,st,4,yr)} + \\ & 9.61 \times \text{FWIND(dir,st,5,yr)} + \\ & 12.52 \times \text{FWIND(dir,st,6,yr)}] \, / \, \text{FWIND2(dir,st)}\end{aligned}$$

(SENES letter 1986-11-04; see Note 3)

Note 1: The FWIND data or averages thereof may be separately sampled at each time step. Alternately averages over several years may be specified as input. The user must specify.

Note 2: Equations were supplied by SENES in a letter (1986-11-04).

Note 3: Inspection of the UTAP2 code has shown that the following logic has also been applied:
UWIND(dir,st) has a minimum value of 0.5.
(BWG, 87-04-06)

RNGMID(dis) - DISTANCE FROM SOURCE TO RECEPTOR [m]. Downward distance from the tailings source to the receptor.

RNGMDA(dis) - EFFECTIVE DISTANCE FROM SOURCE TO RECEPTOR [m]. The effective distance from the source to the receptor allowing for the source being an area, not a point source.

Figure 2.3.3
Calculate DISTANCE FROM SOURCE TO RECEPTOR (RNGMID(dis))
and
EFFECTIVE DISTANCE FROM SOURCE TO RECEPTOR (RNGMDA(dis))

ATAIL - - -> RNGMID(dis) and
RL RNGMDA(dis)

Short Name	Long Name	SI Unit	Source
ATAIL	INITIAL EXPOSED TAILINGS SURFACE AREA	[m^2]	Sampled
RL	RING LIMITS	[m]	Sampled
RNGMID(dis)	DISTANCE FROM SOURCE TO RECEPTOR	[m]	2.3.3
RNGMDA(dis)	EFFECTIVE DISTANCE FROM SOURCE TO RECEPTOR	[m]	2.3.3

for dis = 1,2,3,4,5

$$\text{RNGMID(dis)} = [\text{RL(dis)} + \text{RL(dis+1)}] / 2 \qquad \text{(see Note 3)}$$

$$\text{RNGMDA(dis)} = (2.87 * (\text{ATAIL})^{0.5} + \text{RNGMID(dis)}) \qquad \text{(see Note 2)}$$

Unit check:

$$\text{RNGMDA:} \quad \left([-] * [m^2]^{0.5} + [m] \right) = [m] \qquad \text{(see Note 1)}$$

$$\text{RNGMID:} \quad [m] + [m] = [m]$$

Note 1: 2.87 is defined as dimensionless, SENES Vol. 3, pg. 5-3.

Note 2: The equation for RNGMDA is not explicitly given in SENES Vol. 3 but corresponds to the SENES $(x + x_o)$ where x_o is defined by SENES equation (5.5).

Note 3: The equation for RNGMID was derived from an inspection of the UTAP2 code. The original specifications assumed that RNGMID was a sampled parameter, and there was no reference to RL. The RL parameter does not appear to be referenced in the SENES report. (BWG, 87-04-06)

Figure 2.3.4
Calculate VERTICAL
DISPERSION COEFFICIENT
(VDISP(dis,st))

VDISP(dis,st) - VERTICAL DISPERSION COEFFICIENT [-]. Vertical dispersion coefficient used in the sector-averaged Gaussian plume model for the dispersion of contaminants in the atmosphere.

RNGMID(dis)
RNGMDA(dis)
AW(RNGMID(dis,st)) - - -> VDISP(dis,st)
BW(RNGMID(dis,st))

Short Name	Long Name	SI Unit	Source
AW(RNGMID(dis),st)	VERTICAL DISPERSION LINEAR PARAMETER	[m]	Sampled
BW(RNGMID(dis),st)	VERTICAL DISPERSION EXPONENT PARAMETER	[-]	Sampled
RNGMID(dis)	DISTANCE FROM SOURCE TO RECEPTOR	[m]	2.3.3
RNGMDA(dis)	EFFECTIVE DISTANCE FROM SOURCE TO RECEPTOR	[m]	2.3.3
VDISP(dis,st)	VERTICAL DISPERSION COEFFICIENT	[-]	2.3.4

(a) for dis = 1 to 5, st = 1 to 6

$$\mathrm{VDISP(dis,st)} = \mathrm{AW(RNGMID(dis),st)} * \left(\frac{\mathrm{RNGMDA(dis)}}{(1)}\right)^{\mathrm{BW(RNGMID(dis))st)}}$$

(eqn. 5.6)

where the selected values for AW and BW depend on the distances (RNGMID(dis)). For RNGMDA(dis) > 5000, use AW(2,st) and BW(2,st); otherwise use AW(1,st) and BW(1,st).

(b) If VDISP(dis,st) > 5000 then VDISP(dis,st) = 5000

(below eqn. 5.6)

Unit check:

$$[m] * \left(\frac{[m]}{[1]}\right)^{[-]} = [m]$$

Note: It is assumed AW has the dimensions [m] and BW is dimensionless [-]. The unit check then works only if RNGMIDA is divided by 1.0 [m] in eqn. (5.6).

Figure 2.3.5
Calculate CONC. OF CONTAMINANT IN AIR AT RECEPTOR
(AIRC(nuc,loc), nuc= nat-U, tot-Th, Ra-226, Pb-210, Rn)
(Page 1 of 2)

AIRC(nuc,loc) - CONC. OF CONTAMINANT IN AIR AT RECEPTOR [Bq m^{-3}]. Average annual concentration of radionuclide (nuc= U-nat, Th-tot, Ra-226, Pb-210, Rn-222) associated with dust (or gas) in air at a receptor (loc=1,80).

FWIND2(dir,st)
UWIND(dir,st)
VDISP(dis,st)
RNGMIDA(dis) - - -> AIRC(nuc,loc) <—— EMRATE(nuc)
HSRC EMRATE(Rn)
FWIND1(dis)
FWINDT

FWIND(dir,st,vel,yr) - - -> FWIND1(dis)

Short Name	Long Name	SI Unit	Source
AIRC(nuc,loc)	CONC. OF CONTAMINANT IN AIR AT RECEPTOR	[Bq m^{-3}]	2.3.5
EMRATE(nuc)	ANN. AVG. EMISSION RATE OF RADIONUCLIDES IN DUST FROM TAILINGS	[Bq s^{-1}]	2.1
EMRATE(Rn)	ANN. AVG. EMISSION RATE OF RN GAS FROM TAILINGS	[Bq s^{-1}]	2.2.1
FWIND(dir,st,vel,yr)	FRACTION OF WIND TYPE	[-]	Sampled
FWIND1(dir)	FRACTION OF TIME WIND BLOWS TO RECEPTOR WITH HIGH WIND SPEEDS	[-]	(2.3.5)
FWIND2(dir,st)	FRACTION OF TIME WIND BLOWS TO RECEPTOR	[-]	2.3.1
FWINDT	FRACTION OF TIME WITH HIGH SPEED WINDS	[-]	(2.1)
HSRC	HEIGHT OF SOURCE	[m]	Sampled
RNGMDA(dis)	EFFECTIVE DISTANCE FROM SOURCE TO RECEPTOR	[m]	2.3.3
UWIND(dir,st)	MEAN WIND SPEED, SOURCE TO RECEPTOR	[m s^{-1}]	2.3.2
VDISP(dis,st)	VERTICAL DISPERSION COEFFICIENT	[-]	2.3.4

for each dir (1 to 16) and distance (1 to 5) giving a unique location "loc" and for each nuclide:

$$\text{AIRC(nuc,loc)} = \frac{2.032 * \text{EMRATE(nuc)}}{\text{RNGMDA(dis)}} * \sum_{st=1}^{6}$$

$$\frac{\text{FWIND2(dir,st)} * \text{EXP}\left(\left(\frac{-1}{2}\right)\left(\frac{\text{HSRC}}{\text{VDISP(dis,st)}}\right)^2\right)}{\text{UWIND(dir,st)} * \text{VDISP(dis,st)}}$$

(eqn. 5.1; see Notes 1 and 4)

Unit check:

$$\text{AIRC:}\quad \frac{[-] * [\text{Bq s}^{-1}]}{[\text{m}]} * \sum \frac{[-] * \text{EXP}\left([-] * \left(\frac{[\text{m}]}{[\text{m}]}\right)^2\right)}{[\text{m s}^{-1}] * [\text{m}]} = [\text{Bq m}^{-3}]$$

Figure 2.3.5
Calculate CONC. OF CONTAMINANT IN AIR AT RECEPTOR
(AIRC(nuc,loc), nuc= nat-U, tot-Th, Ra-226, Pb-210, Rn)
(Page 2 of 2)

Note 1: The summation is not indicated in eqn. (5.1) but the concentration must be from a sum of terms for the different stability classes.

Note 2: AIRC is calculated here for 80 locations (16 directions, 5 distances).

Note 3: 2.032 and $\left(\frac{-1}{2}\right)$ are assumed dimensionless.

Note 4: Inspection of the UTAP2 code shows that AIRC should also be multiplied by the factor FWIND1(dir)/(FWINDT*6.0) where

$$\mathrm{FWIND1(dir)} = \sum_{st=1}^{6} \sum_{vel=4}^{6} \mathrm{FWIND(dir,st,vel,yr)}$$

for Ra, Th, U and Pb, and by the factor 1/6 for Rn. It is not clear why these factors differ, and the factor 1/6 is not explained. (BWG, 87-04-06)

AIRC(nuc,81) - CONC. OF CONTAMINANT IN AIR, STUDY AREA AVG. [Bq m^{-3}]. Average annual concentration of contaminant associated with dust (or gas) in air at a receptor (nuc=nat-U, tot-Th, Ra-226, Pb-210, Rn), average over study area (loc≡81).

AIRC(nuc,82) - CONC. OF CONTAMINANT IN AIR, WATERSHED AVG. [Bq m^{-3}]. Average annual concentration of contaminant associated with dust (or gas) in air at a receptor (nuc=nat-U, tot-Th, Ra-226 Pb-210, Rn), average over watershed area (loc≡82).

Figure 2.3.6
Calculate CONC. OF CONTAMINANT IN AIR, WATERSHED AVG. (AIRC(nuc,82))
and
Figure 2.3.7
Calculate CONC. OF CONTAMINANT IN AIR, STUDY AREA AVG. (AIRC(nuc,81))

$$\begin{tikzcd}
\begin{array}{l}\text{WATSHD(loc)}\\ \text{WATSHN}\\ \text{RAREA(dis),TAREA}\end{array} \arrow[r, dashed] & \text{AIRC(nuc,82)} & \text{AIRC(nuc,loc)} \arrow[l] \\
\text{RAREA(dis),TAREA} \arrow[r, dashed] & \text{AIRC(nuc,81)} & \text{AIRC(nuc,loc)} \arrow[l]
\end{tikzcd}$$

Short Name	Long Name	SI Unit	Source
AIRC(nuc,81)	CONC. OF CONTAMINANT IN AIR, STUDY AREA AVG.	[Bq m^{-3}]	2.3.7
AIRC(nuc,82)	CONC. OF CONTAMINANT IN AIR, WATERSHED AVG.	[Bq m^{-3}]	2.3.6
AIRC(nuc,loc)	CONC. OF CONTAMINANT IN AIR AT RECEPTOR	[Bq m^{-3}]	2.3.5
RAREA(dis),TAREA	RING AREAS	[m^2]	2.3.7A
WATSHD(loc)	WATERSHED AREA LOCATIONS	[-]	Sampled
WATSHN	NUMBER WATERSHED LOCATIONS	[-]	Sampled

$$\text{AIRC(nuc,82)} = \left(\sum_{i=1}^{\text{WATSHN}} \text{AIRC(nuc,WATSHD(i))} * \text{RAREA}(d^{**})\right) / \text{WSAREA}$$

$$\text{where WSAREA} = \sum_{i=1}^{\text{WATSHN}} \text{RAREA}(d^{**}) \qquad \text{(see note)}$$

$$\text{AIRC(nuc,81)} = \left(\sum_{loc=1}^{80} \text{AIRC(nuc,loc)} * \text{RAREA}(d^{*})\right) / \text{TAREA} \qquad \text{(see note)}$$

Unit check (both equations):

$$\sum \left([\text{Bq m}^{-3}] * [\text{m}^2]\right) / [\text{m}^2] = [\text{Bq m}^{-3}]$$

Note: These equations are not defined in SENES volume 3. Previous versions to those shown here had been derived from the discussion on page 5-5 and in a letter dated 86-12-11 from SENES. The equations shown here were derived from inspection of the UTAP2 code. The index d^{**} in RAREA has the value INT((WATSHD(i)-1)/16) + 1. The index d^{*} has the value INT((loc-1)/16) + 1 (BWG, 87-04-06).

RAREA(dis) - AREA OF RING dis [m^2].
Annular area of ring dis.
TAREA - TOTAL AREA OF RINGS [m^2].
Total area of the five rings.

Figure 2.3.7A
Calculate RING AREAS

(RAREA(dis), TAREA)

RL(dis) - - -> RAREA(dis),TAREA

Short Name	Long Name	SI Unit	Source
RAREA(dis),TAREA	RING AREAS	[m^2]	2.3.7A
RL(dis)	RING LIMITS	[m]	Sampled

```
for  dis = 1 to 5
        RAREA(dis) = $\pi * [RL(dis+1)^2 - RL(dis)^2] / 16$          (see Note)
```

$$TAREA = \sum_{dis=1}^{5} RAREA(dis) * 16$$

Unit check:

RAREA $[m^2] - [m^2] = [m^2]$
TAREA $\Sigma[m^2] * [-] = [m^2]$

Note: These variables are not defined in the SENES text. Inspection of the UTAP2 code shows that they are defined as shown above, and used to calculate AIRC(nuc,81) and AIRC(nuc,82). RL was also shown to be an input sampled parameter. (BWG, 87-04-06)

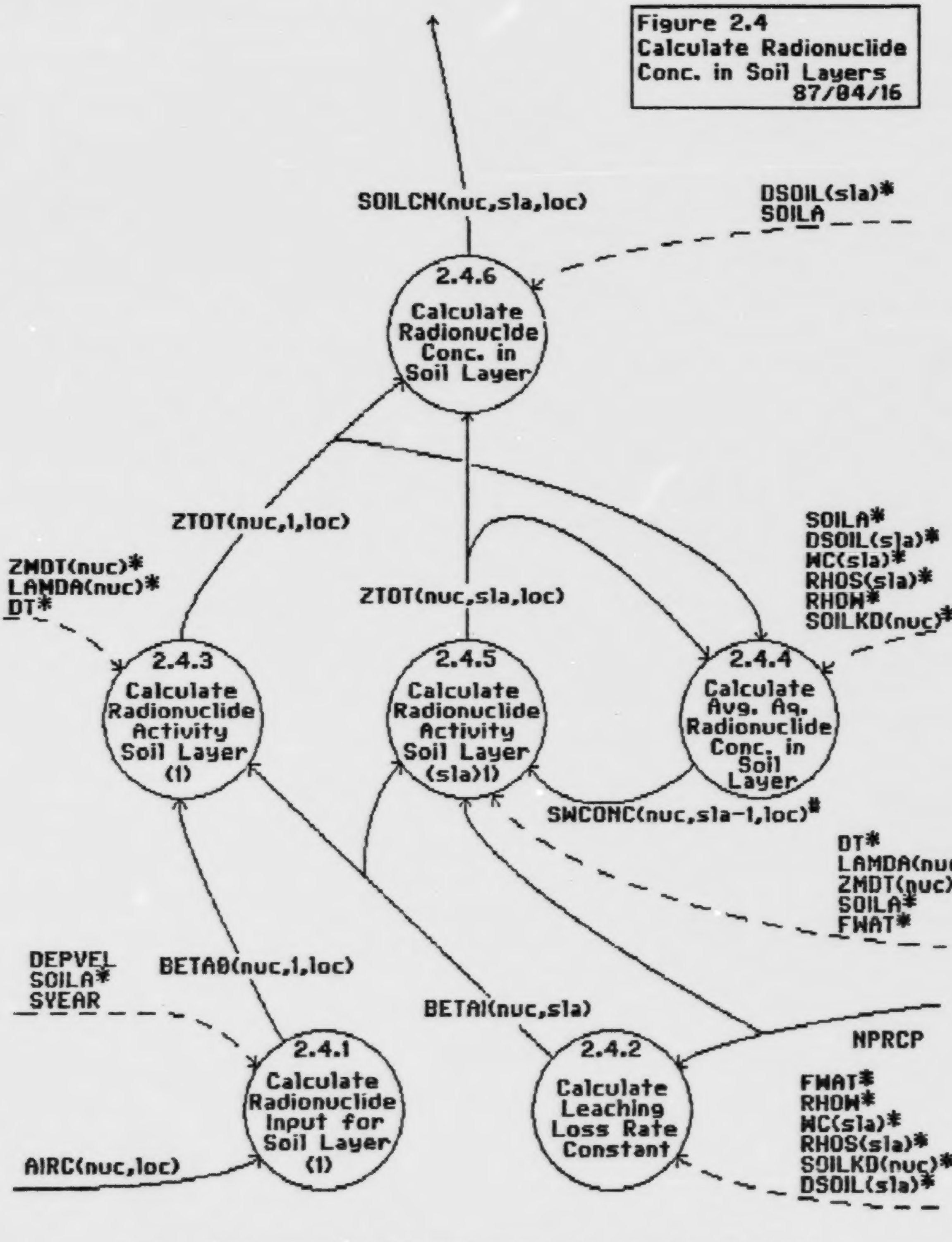


Figure 2.4
Calculate Radionuclide
Conc. in Soil Layers
87/04/16

SOILCN(nuc,sla,loc)
DSOIL(sla)*
SOILA
2.4.6
Calculate Radionuclide Conc. in Soil Layer
ZTOT(nuc,1,loc)
ZMDT(nuc)*
LAMDA(nuc)*
DT*
ZTOT(nuc,sla,loc)
SOILA*
DSOIL(sla)*
WC(sla)*
RHOS(sla)*
RHOW*
SOILKD(nuc)*
2.4.3
Calculate Radionuclide Activity Soil Layer (1)
2.4.5
Calculate Radionuclide Activity Soil Layer (sla)1)
2.4.4
Calculate Avg. Aq. Radionuclide Conc. in Soil Layer
SWCONC(nuc,sla-1,loc)#
DT*
LAMDA(nuc)*
ZMDT(nuc)*
SOILA*
FWAT*
DEPVEL
SOILA*
SYEAR
BETA0(nuc,1,loc)
BETAI(nuc,sla)
NPRCP
2.4.1
Calculate Radionuclide Input for Soil Layer (1)
2.4.2
Calculate Leaching Loss Rate Constant
FWAT*
RHOW*
WC(sla)*
RHOS(sla)*
SOILKD(nuc)*
DSOIL(sla)*
AIRC(nuc,loc)

Note: the value of SWCONC passed to bubble 2.4.5 is the value for the previous soil layer, sla, where sla-1 > 0.

Figure 2.4.1
Calculate RADIONUCLIDE INPUT FOR SOIL LAYER(1)
BETAO(nuc,1,loc)

BETAO(nuc,1,loc) - RADIONUCLIDE INPUT FOR SOIL LAYER(1) [Bq a^{-1}]. Input rate to a soil layer (sla=1,NLAYER) of activity from a radionuclide (nuc),(nuc=Ra-226, Pb-210, tot-Th, nat-U) at a receptor site (loc, loc=1,80).

SYEAR
DEPVEL - - -> BETAO(nuc,1,loc) <—— AIRC(nuc,loc)
SOILA

Short Name	Long Name	SI Unit	Source
AIRC(nuc,loc)	CONC. OF CONTAMINANT IN AIR AT RECEPTOR	[Bq m^{-3}]	2.3.5
BETAO(nuc,1,loc)	RADIONUCLIDE INPUT FOR SOIL LAYER(1)	[Bq a^{-1}]	2.4.1
DEPVEL	DEPOSITION VELOCITY	[m s^{-1}]	Sampled
SOILA	SOIL AREA	[m^2]	Sampled
SYEAR	SECONDS IN A YEAR	[s a^{-1}]	Sampled

BETAO(nuc,1,loc) = AIRC(nuc,loc) * SOILA * DEPVEL * SYEAR
(eqn. 6.11, modified)

Unit check:
BETAO(nuc,1,loc): [Bq m^{-3}] * [m^2] * [m s^{-1}] * [s a^{-1}] = [Bq a^{-1}]

Note 1: BETAO(nuc,1,loc) is calculated for each of the radionuclides "nuc" (nuc= Ra-226, Pb-210, tot-Th, nat-U).

Note 2: Unit inconsistency in that the particle deposition velocity in [m a^{-1}] not [m s^{-1}] is needed, according to the definition on page 6-2. BETAO(nuc,1,luc) must be in [Bq a^{-1}] for consistency in later calculations. The factor SYEAR [s a^{-1}] has been introduced to properly modify eqn. (6.11). (SENES letter 1986-12-02)

Note 3: Inspection of the UTAP2 code shows that SOILA is not included in the code for BETAO. Since SOILA has a constant value of 1.0, its omission does not affect the results. (BWG, 87-04-24)

BETAI(nuc,sla) - LEACHING LOSS RATE CONSTANT [a^{-1}]. The rate constant for the loss of an element (nuc), (nuc=Ra,Pb,Th,U) from a soil layer (sla) by leaching.

Figure 2.4.2
Calculate LEACHING LOSS RATE CONSTANT
(BETAI(nuc,sla))

```
DSOIL(sla)
SOILKD(nuc)
WC(sla)
NPRCP          - - ->  BETAI(nuc,sla)
RHOS(sla)
RHOW
FWAT
```

Short Name	Long Name	SI Unit	Source
BETAI(nuc,sla)	LEACHING LOSS RATE CONSTANT FOR SOIL LAYER	[a^{-1}]	2.4.2
DSOIL(sla)	DEPTH OF SOIL LAYER	[m]	Sampled
FWAT	FRAC. OF NET PPTN. IN RUNOFF	[-]	Sampled
NPRCP	NET PRECIPITATION	[$m\ s^{-1}$]	Sampled
RHOS(sla)	BULK DENSITY OF SOIL LAYER	[$kg\ m^{-3}$]	Sampled
RHOW	WATER DENSITY	[$kg\ m^{-3}$]	Sampled
SOILKD(nuc)	SOIL KD FOR ELEMENT	[$m^3\ kg^{-1}$]	Sampled
WC(sla)	WATER CONTENT OF SOIL LAYER	[-]	Sampled

for sla = 1 to NLAYER

$$\text{BETAI(nuc,sla)} = \text{NPRCP} \,/\, \Big[\text{RHOS(sla)} * \text{DSOIL(sla)} * (\text{WC(sla)}/\text{RHOW} + \text{SOILKD(nuc)})\Big] \quad [a^{-1}]$$

(from eqn. 6.9; see Note 3)

Unit check:

$$\text{BETAI:}\quad [m\ a^{-1}] \,/\, \Big[[kg\ m^{-3}] * [m] * \Big([-] \,/\, [kg\ m^{-3}] + [m^3\ kg^{-1}]\Big)\Big] = [a^{-1}]$$

Note 1: BETAI(nuc,sla) is calculated separately for each soil layer (sla=1, NLAYER) and each of the elements (nuc) nuc = Ra, Pb, Th and U. If SOILKD is location specific, then BETAI is location specific.

Note 2: RHOS(1) and WC(1) are used for the surface layer; RHOS(2) and WC(2) for the subsurface layers.

Note 3: Inspection of the UTAP2 code shows that the above equation is modified, for sla>1, by the multiplicative factor (1-FWAT). This modification has been included in SYVAC3-UT2. (BWG, 87-04-23)

Figure 2.4.3
Calculate RADIONUCLIDE
ACTIVITY SOIL LAYER(1)
(ZTOT(nuc,1,loc))

ZTOT(nuc,1,loc) - RADIONUCLIDE ACTIVITY SOIL LAYER(1) [Bq]. The activity of the radionuclide (nuc) (nuc= Ra-226, Pb-210, tot-Th, nat-U) in the soil layer (sla), (sla=1), at receptor site "loc" at time t.

DT≡Δt
ZMDT(nuc) - - -> ZTOT(nuc,1,loc) <—— BETAO(nuc,1,loc)
LAMDA(nuc) BETAI(nuc,sla)

Short Name	Long Name	SI Unit	Source
BETAI(nuc,sla)	LEACHING LOSS RATE CONSTANT FOR SOIL LAYER	$[a^{-1}]$	2.4.2
BETAO(nuc,1,loc)	RADIONUCLIDE INPUT FOR SOIL LAYER(1)	$[Bq\ a^{-1}]$	2.4.1
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
LAMDA(nuc)	NUCLIDE DECAY CONSTANT	$[a^{-1}]$	Sampled
ZMDT(nuc)	INITIAL RADIONUCLIDE ACTIVITIES IN THE SOIL LAYERS	[Bq]	Sampled
ZTOT(nuc,1,loc)	RADIONUCLIDE ACTIVITY SOIL LAYER(1)	[Bq]	2.4.3

$$ZTOT(nuc,1,loc,-\Delta t) = ZMDT(nuc)$$

$t \geq 0$ solve the following finite difference equations for all "nuc" and "loc":

$$ZTOT(nuc,1,loc,t) = ZTOT(nuc,1,loc,t-\Delta t) * EXP\{-(BETAI(nuc,1) + LAMDA(nuc)) * TIME\} + \frac{BETAO(nuc,1,loc) * \{1-EXP\ \{-(BETAI(nuc,1) + LAMDA(nuc)) * TIME\}}{BETAI(nuc,1) + LAMDA(nuc)}$$

(eqn. 6.8;
see Note 4)

Unit check:

$$[Bq] * EXP\left(([a^{-1}]+[a^{-1}])*[a]\right) + \frac{[Bq\ a^{-1}]*([-]-EXP\{-([a^{-1}]+[a^{-1}])*[a]\})}{([a^{-1}]+[a^{-1}])} = [Bq]$$

Note 1: Values for ZMDT(nuc) = 0 for all nuc (SENES letter 1986-10-15).

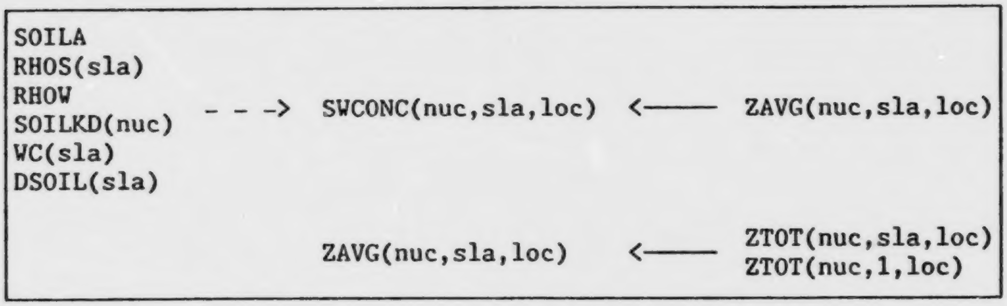
Note 2: In eqn. (6.8) it is assumed that j = sla = 1.

Note 3: Inspection of the UTAP2 code shows that ZTOT is also set to zero at t=0. (BWG, 87-04-06)

Note 4: Inspection of the UTAP2 code shows that the two exponential terms in the above equation have used DT and not TIME in the arguments. SYVAC3-UT2 has been modified accordingly. (BWG, 87-04-23)

SWCONC(nuc,sla,loc) - AVG. AQ. RADIONUCLIDE CONC. IN SOIL LAYER [Bq m^{-3}]. The concentration of the radionuclide (nuc) (nuc = Ra-226, Pb-210, tot-Th, nat-U) partitioned into water in equilibrium with the soil layer at a time that is the average of t and (t-Δt).

Figure 2.4.4
Calculate AVG. AQ.
RADIONUCLIDE CONC. IN
SOIL LAYER
(SWCONC(nuc,sla,loc))



Short Name	Long Name	SI Unit	Source
DSOIL(sla)	DEPTH OF SOIL LAYER	[m]	Sampled
RHOS(sla)	BULK DENSITY OF SOIL LAYER	[kg m^{-3}]	Sampled
RHOW	WATER DENSITY	[kg m^{-3}]	Sampled
SOILA	SOIL AREA	[m^2]	Sampled
SOILKD(nuc)	SOIL KD FOR ELEMENT	[m^3 kg^{-1}]	Sampled
SWCONC(nuc,sla,loc)	AVG. AQ. RADIONUCLIDE CONC. IN SOIL LAYER	[Bq m^{-3}]	2.4.4
WC(sla)	WATER CONTENT OF SOIL LAYER	[-]	Sampled
ZAVG(nuc,sla,loc)	AVG. ACTIVITY IN SOIL LAYER	[Bq]	(2.4.4)
ZTOT(nuc,1,loc)	RADIONUCLIDE ACTIVITY SOIL LAYER(1)	[Bq]	2.4.3
ZTOT(nuc,sla,loc)	RADIONUCLIDE ACTIVITY SOIL LAYER (sla≥2)	[Bq]	2.4.5

$$\text{ZAVG(nuc,sla,loc)} = \Big[\text{ZTOT(nuc,sla,loc,t)} + \text{ZTOT(nuc,sla,loc,t-}\Delta\text{t)}\Big] \;/\; 2 \qquad \text{(eqn. 6.10)}$$

$$\text{SWCONC(nuc,sla,loc)} =$$

$$\text{ZAVG(nuc,sla,loc)} \;/\; [\text{RHOS(sla)} * \text{SOILA} * \text{DSOIL(sla)} * \left(\frac{\text{WC(sla)}}{\text{RHOW}} + \text{SOILKD(nuc)}\right) \qquad \text{(eqn. 6.5)}$$

Unit check: ZAVG ([Bq] + [Bq]) / [-] = [Bq]

$$\text{SWCONC} \quad [\text{Bq}] \;/\; \left([\text{kg m}^{-3}] * [\text{m}^2] * [\text{m}] * \left(\frac{[-]}{[\text{kg m}^{-3}]} + [\text{m}^3\ \text{kg}^{-1}]\right)\right) = [\text{Bq m}^{-3}]$$

Note 1: The value of SWCONC(nuc,1,loc) is requireed for the calculation of SWCONC(nuc,2,loc) at each time step (and similarly for any lower layers the water concentration in the next higher layer would be required).

Note 2: It is assumed Z_1 in eqn. (6.5) is ZAVG.

Note 3: Inspection of the UTAP2 code shows that SOILA is missing from the coding for ZAVG. Since its value is a constant 1.0, however, the results should not be affected. (BWG, 87-04-23)

Figure 2.4.5
Calculate RADIONUCLIDE ACTIVITY SOIL LAYER $(sla \geq 2)$ (ZTOT(nuc,sla,loc), $(sla \geq 2)$)
(Page 1 of 2)

ZTOT(nuc,sla,loc),$(sla \geq 2)$ - RADIONUCLIDE ACTIVITY SOIL LAYER $(sla \geq 2)$ [Bq]. The activity of the radionuclide (nuc) (nuc= Ra-226, Pb=210, tot-Th, nat-U) in the soil layer (sla) (sla=2, WLAYER) at receptor site "loc" at time t.

```
DT≡Δt
ZMDT(nuc)     - - ->  ZTOT(nuc,sla,loc)  <———  BETAO(nuc,sla,loc)
LAMDA(nuc)                                     BETAI(nuc,sla)

SOILA                                          NPRCP
FWAT          - - ->  BETAO(nuc,sla,loc) <———  SWCONC(nuc,sla-1,loc)
```

Short Name	Long Name	SI Unit	Source
BETAI(nuc,sla)	LEACHING LOSS RATE CONSTANT	$[a^{-1}]$	2.4.2
BETAO(nuc,sla,loc)	RADIONUCLIDE INPUT FOR SOIL LAYER $(sla \geq 2)$	$[Bq\ a^{-1}]$	(2.4.5)
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
FWAT	FRAC. OF NET PPTN. IN RUNOFF	[-]	Sampled
LAMDA(nuc)	NUCLIDE DECAY CONSTANT	$[a^{-1}]$	Sampled
NPRCP	NET PRECIPITATION	$[m\ a^{-1}]$	Sampled
SOILA	SOIL AREA	$[m^2]$	Sampled
SWCONC(nuc,sla-1,loc)	AVG. AQ. RADIONUCLIDE CONC. IN SOIL LAYER (sla-1) $(sla \geq 2)$	$[Bq\ m^{-3}]$	2.4.4
ZMDT(nuc)	INITIAL RADIONUCLIDE ACTIVITIES IN THE SOIL LAYERS	[Bq]	Sampled
ZTOT(nuc,sla,loc)	RADIONUCLIDE ACTIVITY SOIL LAYER $(sla \geq 2)$	[Bq]	2.4.5

for sla > 1 and for nuc = Ra-226, Pb-210, tot-Th and nat-U and for all loc:

$$\text{BETAO(nuc,sla,loc)} = \text{SWCONC(nuc,sla-1,loc)} * \text{NPRCP} * \text{SOILA} * (1-\text{FWAT}) \qquad \text{(eqn. 6.12)}$$

then solve the finite difference equations for all "nuc" and "loc" for the particular soil layer $sla \geq 2$.

$$\text{ZTOT}(\text{nuc,sla,loc},-\Delta t) = \text{ZMDT(nuc)} \qquad \text{(SENES letter, 1986-12-02)}$$

For $t \geq 0$

$$\text{ZTOT(nuc,sla,loc,t)} = \text{ZTOT}(\text{nuc,sla,loc},t-\Delta t) * \text{EXP}\ \{-(\text{BETAI(nuc,sla)} + \text{LAMDA(nuc)}) * \text{TIME}\} + \frac{\text{BETAO(nuc,sla,loc)} * \{1-\text{EXP}\{-(\text{BETAI(nuc,sla)} + \text{LAMDA(nuc)}) * \text{TIME}\}}{\text{BETAI(nuc,sla)} + \text{LAMDA(nuc)}}$$

(eqn. 6.8)

Unit check:

$$\text{BETAO} \quad [Bq\ m^{-3}] * [m\ a^{-1}] * [m^2] * ([-] - [-]) = [Bq\ a^{-1}]$$

$$\text{ZTOT} \quad [Bq] * \text{EXP}\ (([a^{-1}] + [a^{-1}] * [a]) + \frac{[Bq\ a^{-1}] * ([-] - \text{EXP}(([a^{-1}] + [a^{-1}] * [a]))}{([a^{-1}] + [a^{-1}])} = [Bq]$$

Figure 2.4.5
Calculate RADIONUCLIDE ACTIVITY SOIL LAYER (sla$\geq$2) (ZTOT(nuc,sla,loc), (sla$\geq$2))
(Page 2 of 2)

Note 1: "1" in equation (6.12) is assumed to be dimensionless.

Note 2: Inspection of the UTAP2 code shows that SOILA is missing from the coding for BETAO. Since its value is a constant 1.0, however, the results should not be affected. (BWG, 87-04-23)

Note 3: Inspection of the UTAP2 code shows that the exponential terms involving TIME have instead involved DT (in two places). SYVAC3-UT2 has been modified accordingly. (BWG, 87-04-23)

Figure 2.4.6
Calculate RADIONUCLIDE
CONC. IN SOIL LAYER
(SOILCN(nuc,sla,loc))

SOILCN(nuc,sla,loc) - RADIONUCLIDE CONC. IN SOIL LAYER [Bq m^{-3}]. The concentration of the radionuclide (nuc) (nuc= Ra-226, Pb-210, tot-Th, nat-U) in a particular soil layer "sla (sla=1,NLAYER)" at receptor location "loc" as a function of time.

SOILA
DSOIL(sla) - - -> SOILCN(nuc,sla,loc) <—— ZTOT(nuc,sla,loc)
ZTOT(nuc,1,loc)

Short Name	Long Name	SI Unit	Source
DSOIL(sla)	DEPTH OF SOIL LAYER	[m]	Sampled
SOILA	SOIL AREA	[m^2]	Sampled
SOILCN(nuc,sla,loc)	RADIONUCLIDE CONC. IN SOIL LAYER	[Bq m^{-3}]	2.4.6
ZTOT(nuc,1,loc)	RADIONUCLIDE ACTIVITY SOIL LAYER(1)	[Bq]	2.4.3
ZTOT(nuc,sla,loc)	RADIONUCLIDE ACTIVITY SOIL LAYER (sla≥2)	[Bq]	2.4.5

SOILCN(nuc,sla,loc) = ZTOT(nuc,sla,loc) / (DSOIL(sla) * SOILA)
(see Note 1)

Unit check:

$$[Bq] / ([m] * [m^2]) = [Bq\ m^{-3}]$$

Note 1: The equation was supplied in a SENES letter dated 1987-02-03.

Note 2: Inspection of the UTAP2 code shows that SOILA is missing from the coding for SOILCN. Since it has a constant value of 1.0, however, the results should not be affected. (BWG, 87-04-23)

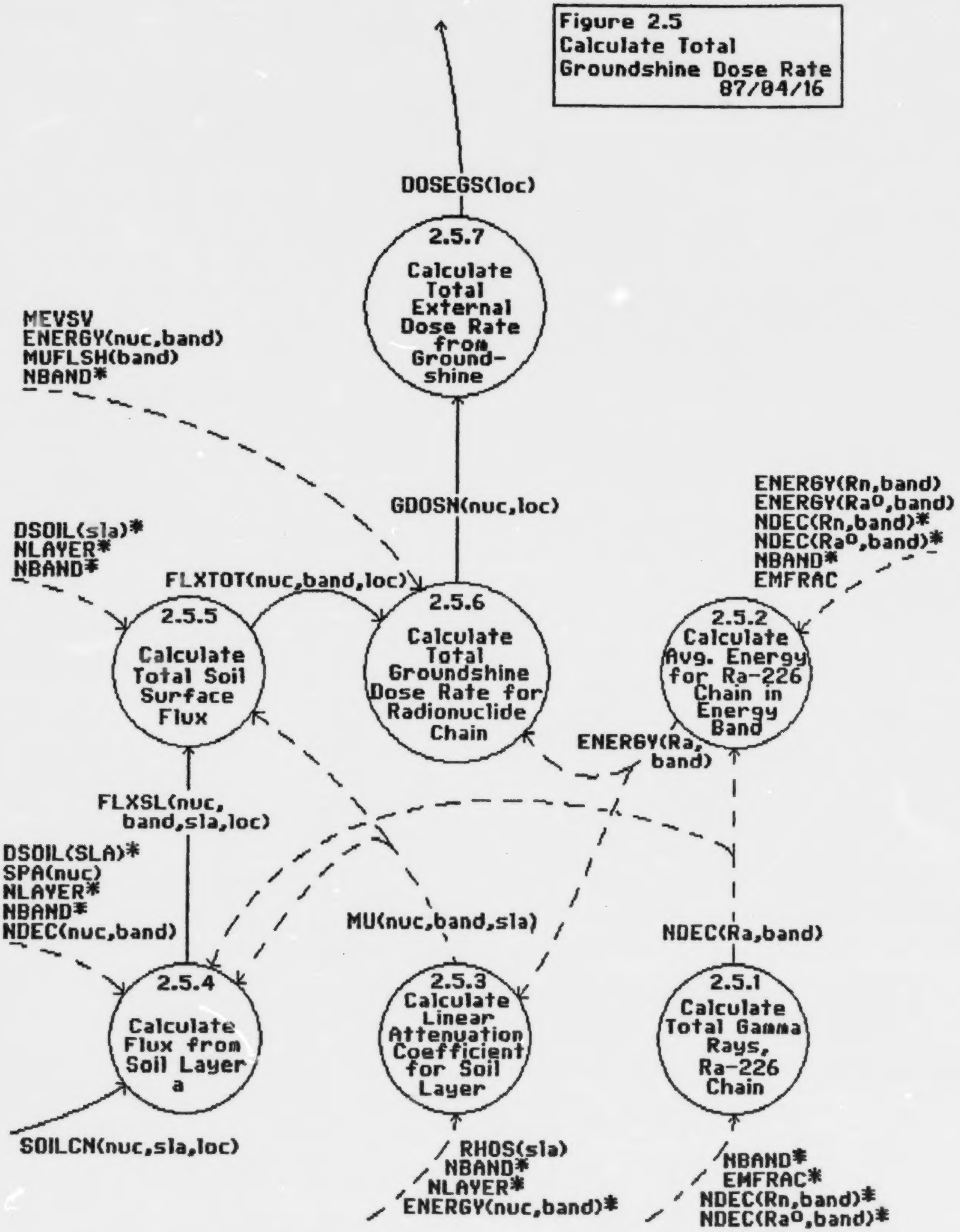

DOSEGS(loc)
2.5.7
Calculate Total External Dose Rate from Groundshine
MEVSV
ENERGY(nuc,band)
MUFLSH(band)
NBAND*
GDOSN(nuc,loc)
ENERGY(Rn,band)
ENERGY(Ra0,band)
NDEC(Rn,band)*
NDEC(Ra0,band)*
NBAND*
EMFRAC
DSOIL(sla)*
NLAYER*
NBAND*
FLXTOT(nuc,band,loc)
2.5.5
Calculate Total Soil Surface Flux
2.5.6
Calculate Total Groundshine Dose Rate for Radionuclide Chain
2.5.2
Calculate Avg. Energy for Ra-226 Chain in Energy Band
ENERGY(Ra, band)
FLXSL(nuc, band,sla,loc)
DSOIL(SLA)*
SPA(nuc)
NLAYER*
NBAND*
NDEC(nuc,band)
MU(nuc,band,sla)
NDEC(Ra,band)
2.5.4
Calculate Flux from Soil Layer a
2.5.3
Calculate Linear Attenuation Coefficient for Soil Layer
2.5.1
Calculate Total Gamma Rays, Ra-226 Chain
SOILCN(nuc,sla,loc)
RHOS(sla)
NBAND*
NLAYER*
ENERGY(nuc,band)*
NBAND*
EMFRAC*
NDEC(Rn,band)*
NDEC(Ra0,band)*

Figure 2.5
Calculate Total
Groundshine Dose Rate
87/04/16

Note: for ENERGY(nuc,band) and NDEC(nuc,band), nuc=U, Th and Pb.

Figure 2.5.1
Calculate TOTAL GAMMA RAYS, RA-226 CHAIN (NDEC(Ra,band))

NDEC(Ra,band) - TOTAL GAMMA RAYS, RA-226 CHAIN $[\gamma\text{-rays kg}^{-1}\text{ s}^{-1}]$. Total number of gamma rays per second in a particular energy band from any specified radionuclide decay chain.

NDEC(Rn,band)
NBAND
NDEC(Ra°,band) - - -> NDEC(Ra,band)
EMFRAC

Short Name	Long Name	SI Unit	Source
EMFRAC	EMANATION COEFFICIENT SOIL	[-]	Sampled
NBAND	NUMBER OF ENERGY BANDS	[-]	Sampled
NDEC(Ra,band)	TOTAL GAMMA RAYS, RA-226 CHAIN	$[\gamma\text{ kg}^{-1}\text{ s}^{-1}]$	2.5.1
NDEC(Ra°,band)	TOTAL GAMMA RAYS, RA-226 ONLY	$[\gamma\text{ kg}^{-1}\text{ s}^{-1}]$	Sampled
NDEC(Rn, band)	TOTAL GAMMA RAYS, RN	$[\gamma\text{ kg}^{-1}\text{ s}^{-1}]$	Sampled

for all bands from 1 to NBAND

$$\text{NDEC(Ra,band)} = \text{NDEC(Ra}^{\circ}\text{,band)} + \text{NDEC(Rn,band)} * (1-\text{EMFRAC})$$

(eqn. 7.8; see Note 1)

Unit check:

$$[\gamma\text{-rays kg}^{-1}\text{ s}^{-1}] + [\gamma\text{-rays kg}^{-1}\text{ s}^{-1}] * ([-] - [-])$$
$$= [\gamma\text{-rays kg}^{-1}\text{ s}^{-1}]$$

Note 1: Equation confirmed in a letter from SENES (1987-02-03).

Note 2: "1" in the equation is assumed dimensionless.

Note 3: Ra° ≡ Radium-226 only.

ENERGY(Ra,band) - AVG. ENERGY FOR RA-226 CHAIN IN ENERGY BAND [MeV]. The average decay energy in a particular energy band for the Ra-226 decay chain.

Figure 2.5.2
Calculate AVG. ENERGY FOR RA-226 CHAIN IN ENERGY BAND (ENERGY(Ra,band))

```
NDEC(Ra,band)
ENERGY(Ra°,band)
NBAND
ENERGY(Rn,band)   - - ->  ENERGY(Ra,band)
EMFRAC
NDEC(Rn,band)
NDEC(Ra°,band)
```

Short Name	Long Name	SI Unit	Source
EMFRAC	EMANATION COEFFICIENT SOIL	[-]	Sampled
ENERGY(Ra,band)	AVG. ENERGY FOR RA-226 CHAIN IN ENERGY BAND	[MeV]	2.5.2
ENERGY(Ra°,band)	AVG. ENERGY FOR RA-226 IN ENERGY BAND	[MeV]	Sampled
ENERGY(Rn,band)	AVG. ENERGY FOR RN CHAIN IN ENERGY BAND	[MeV]	Sampled
NBAND	NUMBER OF ENERGY BANDS	[-]	Sampled
NDEC(Ra,band)	TOTAL GAMMA RAYS, RA-226 CHAIN	$[\gamma\ kg^{-1}\ s^{-1}]$	2.5.1
NDEC(Ra°,band)	TOTAL GAMMA RAYS, RA ONLY	$[\gamma\ kg^{-1}\ s^{-1}]$	Sampled
NDEC(Rn,band)	TOTAL GAMMA RAYS, RN	$[\gamma\ kg^{-1}\ s^{-1}]$	Sampled

Calculate for all bands from 1 to NBAND

$$\mathrm{ENERGY(Ra,band)} = \Big[\mathrm{ENERGY(Ra^{\circ},band)} * \mathrm{NDEC(Ra^{\circ},band)} + \mathrm{ENERGY(Rn,band)} * \mathrm{NDEC(Rn,band)} * (1-\mathrm{EMFRAC})\Big] \,/\, \mathrm{NDEC(Ra,band)}$$

(eqn. 7.9; see Note 1)

Unit check:

$$\frac{[\mathrm{MeV}] * [\gamma\ \mathrm{kg}^{-1}\ \mathrm{s}^{-1}] + [\mathrm{MeV}] * [\gamma\ \mathrm{kg}^{-1}\ \mathrm{s}^{-1}] * ([-] - [-])}{[\gamma\ \mathrm{kg}^{-1}\ \mathrm{s}^{-1}]} = [\mathrm{MeV}]$$

Note 1: The modified form of this equation and the definitions have been confirmed by SENES in a letter (1987-02-03).

Note 2: Ra° ≡ Radium-226 only.

Figure 2.5.3
Calculate LINEAR ATTENUATION COEFFICIENT FOR SOIL LAYER (MU(nuc,band,sla))

MU(nuc,band,sla) - LINEAR ATTENUATION COEFFICIENT FOR SOIL LAYER [m^{-1}]. The energy dependent attenuation coefficient for a particular soil layer, set equal to the absorption coefficient.

ENERGY(nuc,band)
ENERGY(Ra,band)
NLAYER - - -> MU(nuc,band,sla)
NBAND
RHOS(sla)

Short Name	Long Name	SI Unit	Source
ENERGY(nuc,band)	AVG. ENERGY FOR RADIONUCLIDE CHAIN IN ENERGY BAND	[MeV]	Sampled
ENERGY(Ra,band)	AVG. ENERGY FOR RA-226 CHAIN IN ENERGY BAND	[MeV]	2.5.2
MU(nuc,band,sla)	LINEAR ATTENUATION COEFFICIENT FOR SOIL LAYER	[m^{-1}]	2.5.3
NBAND	NUMBER OF ENERGY BANDS	[-]	Sampled
NLAYER	NUMBER OF SOIL LAYERS	[-]	Sampled
RHOS(sla)	BULK DENSITY OF SOIL LAYER	[kg m^{-3}]	Sampled

Calculate for nuc = U, Th, Pb, Ra(total), band = 1 to NBAND and sla = 1 to NLAYER

MU(nuc,band,sla)

$$= 2.7 * 10^{-3} * \left[\frac{\text{ENERGY(nuc,band)}}{1.0}\right]^{-0.320} * \text{RHOS(sla)} \qquad \text{(eqns. 7.10 \& 7.11)}$$

Unit check:

$$[m^2\ kg^{-1}] * \left(\frac{[MeV]}{[MeV]}\right)^{[-]} * [kg\ m^{-3}] = [m^{-1}]$$

Note 1: The energy (ENERGY(nuc,band)) is assumed to be divided by 1.0 [MeV] to maintain the unit check.

Note 2: The units of $2.7 * 10^{-3}$ are assumed to be [$m^2\ kg^{-1}$].

Figure 2.5.4
Calculate FLUX FROM A SOIL LAYER
(FLXSL(nuc,band,sla,loc))

FLXSL(nuc,band,sla,loc) - FLUX FROM A SOIL LAYER [γ-rays m^{-2} s^{-1}]. The γ-flux in a particular energy band (band=1,NBAND) from a particular decay chain (U-238, nat-Th, Ra-226, Pb-210) for a particular soil layer (sla=1,NLAYER).

MU(nuc,band,sla)
NDEC(Ra,band)
NDEC(nuc,band)
MUD(nuc,band,sla) - - -> FLXSL (nuc,band,sla,loc) <—— SOILCN(nuc,sla,loc)
SPA(nuc)
NLAYER
NBAND

MU(nuc,band,sla)
DSOIL(sla
NLAYER - - -> MUD(nuc,band,sla)
NBAND

Short Name	Long Name	SI Unit	Source
DSOIL(sla)	DEPTH OF SOIL LAYER	[m]	Sampled
FLXSL(nuc,band,sla,loc)	FLUX FROM A SOIL LAYER	[γ m^{-2} s^{-1}]	2.5.4
MU(nuc,band,sla)	LINEAR ATTENUATION COEFFICIENT FOR SOIL LAYER	[m^{-1}]	2.5.3
MUD(nuc,band,sla)	ATTENUATION PRODUCT	[-]	(2.5.4)
NBAND	NUMBER OF ENERGY BANDS	[-]	Sampled
NDEC(nuc,band)	TOTAL GAMMA RAYS, NUCLIDE	[γ kg^{-1} s^{-1}]	Sampled
NDEC(Ra,band)	TOTAL GAMMA RAYS, RA-226 CHAIN	[γ kg^{-1} s^{-1}]	2.5.1
NLAYER	NUMBER OF SOIL LAYERS	[-]	Sampled
SOILCN(nuc,sla,loc)	RADIONUCLIDE CONC. IN SOIL LAYER	[Bq m^{-3}]	2.4.6
SPA(nuc)	RADIONUCLIDE SPECIFIC ACTIVITY	[Bq kg^{-1}]	Sampled

For nuc = U, Th, Ra-226, Pb-210; band = 1 to NBAND; sla = 1 to NLAYER; and loc = 1 to 80:

$$\mathrm{MUD(nuc,band,sla)} = \mathrm{MU(nuc,band,sla)} * \mathrm{DSOIL(sla)}$$

$$\begin{aligned}\mathrm{FLXSL(nuc,band,sla,loc)} &= \frac{\mathrm{SOILCN(nuc,sla,loc)} * \mathrm{NDEC(nuc,band)}}{2 * \mathrm{SPA(nuc)} * \mathrm{MU(nuc,band,sla)}} * \\ &\Big[1.0 - \mathrm{EXP}[-\mathrm{MUD(nuc,band,sla)}] - \mathrm{MUD(nuc,band,sla)} * \\ &\Big\{\gamma + \ln(\mathrm{MUD(nuc,band,sla)}) - \mathrm{MUD(nuc,band,sla)} + \frac{(\mathrm{MUD(nuc,band,sla)})^2}{2^2} \\ &- \frac{(\mathrm{MUD(nuc,band,sla)})^3}{3^2} + \ldots\Big\}\Big] \end{aligned} \qquad \text{(eqn. 7.3)}$$

Unit check:

$$\mathrm{MUD} \quad [m^{-1}] * [m] = [-]$$

$$\begin{aligned}\mathrm{FLXSL} \quad &\frac{[\mathrm{Bq}\ m^{-3}] * [\gamma\ kg^{-1}\ s^{-1}]}{[-] * [\mathrm{Bq}\ kg^{-1}] * [m^{-1}]} * \Big[[-] - \exp[-] - [-] * \\ &\Big\{[-] + [-] - [-] + \frac{[-]^2}{[-]^2} - \frac{[-]^3}{[-]^3} + \ldots\Big\}\Big] = [\gamma\text{-rays } m^{-2}\ s^{-1}]\end{aligned}$$

Note 1: γ in eqn. (7.3) is a constant equal to 0.5772157.
Note 2: 2 (in denominator of first term), γ, 2^2, 3^2, etc. are assumed to be dimensionless.
Note 3: It is not known what term truncates the series.

Figure 2.5.5
Calculate TOTAL SOIL
SURFACE FLUX
(FLXTOT(nuc,band,loc))

FLXTOT(nuc,band,loc) - TOTAL SOIL SURFACE FLUX [γ-rays m^{-2} s^{-1}]. The total γ-flux in a particular energy band (band=1,NBAND) at the soil surface from a specific decay chain (nuc=U, Th, Ra-226, Pb-210).

DSOIL(sla)
NBAND
MU(nuc,band,sla) - - -> FLXTOT (nuc,band,loc) <—— FLXSL(nuc,band,sla,loc)
NLAYER

Short Name	Long Name	SI Unit	Source
DSOIL(sla)	DEPTH OF SOIL LAYER	[m]	Sampled
FLXSL(nuc,band,sla,loc)	FLUX FROM A SOIL LAYER	[γ m^{-2} s^{-1}]	2.5.4
FLXTOT(nuc,band,loc)	TOTAL SOIL SURFACE FLUX	[γ m^{-2} s^{-1}]	2.5.5
MU(nuc,band,sla)	LINEAR ATTENUATION COEFFICIENT FOR SOIL LAYER	[m^{-1}]	2.5.3
NBAND	NUMBER OF ENERGY BANDS	[-]	Sampled
NLAYER	NUMBER OF SOIL LAYERS	[-]	Sampled

Calculate for nuc = U, Th, Ra-226, Pb-210; band = 1 to NBAND; and loc = 1 to 80:

$$\mathrm{FLXTOT(nuc,band,sla)} = \mathrm{FLXSL(nuc,band,1,loc)} + \sum_{\mathrm{sla}=2}^{\mathrm{NLAYER}} \mathrm{FLXSL(nuc,band,sla,loc)} * \prod_{k=1}^{\mathrm{sla}-1} \mathrm{EXP}\left(-\mathrm{MU(nuc,band,sla)} * \mathrm{DSOIL(sla)}\right)$$

(eqn. 7.12)

Unit check:

$$[\gamma\ m^{-2}\ s^{-1}] + \Sigma[\gamma\ m^{-2}\ s^{-1}] * \pi\ \mathrm{EXP}([m^{-1}] * [m]) = [\gamma\ m^{-2}\ s^{-1}]$$

Figure 2.5.6
Calculate TOTAL
GROUNDSHINE DOSE RATE
FOR RADIONUCLIDE CHAIN
(GDOSN(nuc,loc))

GDOSN(nuc,loc) - TOTAL GROUNDSHINE DOSE RATE FOR RADIONUCLIDE CHAIN [Sv a^{-1}]. Total groundshine dose rate at a receptor (loc=1,80) from a radionuclide decay chain (nuc= U-238, tot-Th, Ra-226(total), Pb-210).

NBAND - - -> GDOSN(nuc,loc) <—— GDOS(nuc,band,loc)

MUFLSH(band)
ENERGY(nuc,band)
ENERGY(Ra,band) - - -> GDOS(nuc,band,loc) <—— FLXTOT(nuc,band,loc)
MEVSV
NBAND

Short Name	Long Name	SI Unit	Source
GDOS(nuc,band,loc)	BAND GROUNDSHINE DOSE	[Sv a^{-1}]	(2.5.6)
GDOSN(nuc,loc)	TOTAL GROUNDSHINE DOSE RATE FOR RADIONUCLIDE CHAIN	[Sv a^{-1}]	2.5.6
ENERGY(nuc,band)	AVG. ENERGY FOR RADIONUCLIDE CHAIN IN ENERGY BAND	[MeV]	Sampled
ENERGY(Ra,band)	AVG. ENERGY FOR RA-226 CHAIN IN ENERGY BAND	[MeV]	2.5.2
FLXTOT(nuc,band,loc)	TOTAL SOIL SURFACE FLUX	[γ m^{-2} s^{-1}]	2.5.5
MEVSV	GROUNDSHINE CONVERSION FACTOR	[Sv kg s γ^{-1} a^{-1}]	Sampled
MUFLSH(band)	TISSUE MASS ENERGY ABSORPTION COEFFICIENT	[m^2 kg^{-1}]	Sampled
NBAND	NUMBER OF ENERGY BANDS	[-]	Sampled

For nuc = U, Th, Ra, Pb; band = 1 to NBAND, and loc = 1 to 80:

$$\text{GDOS(nuc,band,loc)} = \text{FLXTOT(nuc,band,loc)} * \text{ENERGY(nuc,band)} * \text{MUFLSH(band)} * \text{MEVSV} \qquad \text{(eqn. 7.13)}$$

For nuc = U, Th, Ra, Pb; and loc = 1 to 82:

$$\text{GDOSN(nuc,loc)} = \sum_{1}^{\text{NBAND}} \text{GDOS(nuc,band,loc)} \qquad \text{(eqn on pg. 7-10)}$$

Unit check: GDOS: band =

$$[\gamma\ m^{-2}\ s^{-1}] * [MeV] * [m^2\ kg^{-1}] * [Sv\ a^{-1}\ MeV^{-1}\ kg\ s\ \gamma^{-1}] = [Sv\ a^{-1}]$$

$$\text{GDOSN: } \Sigma[Sv\ a^{-1}] = [Sv\ a^{-1}]$$

Note: Units of MEVSV are assumed based on a sentence in an earlier draft of the SENES documentation.

Figure 2.5.7
Calculate TOTAL EXTERNAL DOSE RATE FROM GROUNDSHINE (DOSEGS(loc))

DOSEGS(loc) - TOTAL EXTERNAL DOSE RATE FROM GROUNDSHINE [Sv a^{-1}]. Total groundshine dose rate at the receptor locations (loc=1,80) summed over all decay chains (U-238, Th-tot, Ra-226(total), Pb-210).

$$\boxed{\text{GDOSN(nuc,loc)} \longrightarrow \text{DOSEGS(loc)}}$$

Short Name	Long Name	SI Unit	Source
DOSEGS(loc)	TOTAL EXTERNAL DOSE RATE FROM GROUNDSHINE	[Sv a^{-1}]	2.5.7
GDOSN(nuc,loc)	GROUNDSHINE DOSE RATE FOR RADIONUCLIDE CHAIN	[Sv a^{-1}]	2.5.6

For loc = 1,80:

$$\text{DOSEGS(loc)} = \sum_{\text{nuc}} \text{GDOSN(nuc,loc)} \qquad \text{for nuc} = \text{U, Th, Ra, Pb}$$

Unit check: $\Sigma[\text{Sv a}^{-1}] = [\text{Sv a}^{-1}]$

Note: Equation is not given by SENES. It would be more reasonable if the total external dose were (DOSEGS(loc) x OF) where OF is the occupancy factor defined in the DOSE module. The SENES documentation makes no mention of such a calculation, and it has been assumed the total groundshine dose was calculated and used for each full year.

Figure 2.6
Calculate CONC. OF
RADIONUCLIDE IN
VEGETATION
(CVEG(nuc,v,loc))
(Page 1 of 2)

CVEG(nuc,v,loc) - CONC. OF RADIONUCLIDE IN VEGETATION [Bq g^{-1} (wet weight)]. Average annual concentration of a radionuclide (nuc= nat-U, tot-Th, Ra-226, Pb-210) in vegetation of type v (types v = 1,2,3,4,5 are above-ground and below-ground vegetables, summer forage, browse and lichen respectively). The values are calculated at receptor locations - the specific sector and ring locations (1-80) for vegetables, the total area for browse and lichens, and the watershed area for summer forage.

```
DEPVEL
FDEPSF(v)
FDEPED(v)
YDEN(v)                                          AIRC(nuc,loc)
DUREXP(v)     - - ->  CVEG(nuc,v,loc)  <-----   SOILC(nuc,loc)
VEGLEM(v)
DRYRHO
SPTC(nuc,v)

                      SOILC(nuc,loc)   <-----   SOILCN(nuc,sla,loc)

RHOS(sla)     - - ->  DRYRHO
```

Short Name	Long Name	SI Unit	Source
AIRC(nuc,loc)	CONC. OF CONTAMINANT IN AIR AT RECEPTOR	[Bq m^{-3}]	2.3.5, 2.3.6, 2.3.7
CVEG(nuc,v,loc)	CONC. OF RADIONUCLIDE IN VEGETATION	[Bq g^{-1}]	2.6
DEPVEL	DEPOSITION VELOCITY	[m s^{-1}]	Sampled
DRYRHO	DRY SOIL DENSITY	[g m^{-3}]	(2.6)
DUREXP(v)	DURATION OF EXPOSURE OF VEGETATION	[s]	Sampled
FDEPED(v)	FRACTION ON EDIBLE PORTION	[-]	Sampled
FDEPSF(v)	FRACTION OF DEPOSITION RETAINED	[-]	Sampled
RHOS(sla)	BULK DENSITY OF SOIL LAYER	[kg m^{-3}]	Sampled
SOILC(nuc,loc)	RADIONUCLIDE CONC. IN ROOT SOIL LAYER	[Bq m^{-3}]	(2.6)
SOILCN(nuc,sla,loc)	RADIONUCLIDE CONC. IN SOIL LAYER	[Bq m^{-3}]	2.4.6
SPTC(nuc,v)	SOIL-PLANT TRANSFER COEFFICIENT	[-]	Sampled
VEGLAM(v)	WEATHERING LOSS DECAY RATE	[s^{-1}]	Sampled
YDEN(v)	YIELD DENSITY	[g m^{-2}]	Sampled

$$\mathrm{DRYRHO} = \mathrm{RHOS}(2) * 1000 \qquad \text{(SENES letter 1986-10-15)}$$

$$\mathrm{SOILC}(nuc,loc) = \mathrm{SOILCN}(nuc,2,loc) \qquad \text{(SENES letter 1986-10-15)}$$

$$\mathrm{CVEG}(nuc,v,loc) = \mathrm{AIRC}(nuc,loc) * \mathrm{DEPVEL} * \mathrm{FDEPSF}(v) * \mathrm{FDEPED}(v) * \left\{\frac{1-\mathrm{EXP}[-\mathrm{VEGLAM}(v) * \mathrm{DUREXP}(v)]}{\mathrm{YDEN}(v) * \mathrm{VEGLAM}(v)}\right\} + \frac{\mathrm{SPTC}(nuc,v) * \mathrm{SOILC}(nuc,loc)}{\mathrm{DRYRHO}}$$

(eqn 8.1)

Figure 2.6
Calculate CONC. OF
RADIONUCLIDE IN
VEGETATION
(CVEG(nuc,v,loc))
(Page 2 of 2)

Unit check:

DRYRHO: $[\text{kg m}^{-3}] * [\text{g kg}^{-1}] = [\text{g m}^{-3}]$

SOILC: $[\text{Bq m}^{-3}] = [\text{Bq m}^{-3}]$

$$\text{CVEG:}\quad \frac{[\text{Bq m}^{-3}] * [\text{m s}^{-1}] * [-] * [-]}{[\text{g(wet weight) m}^{-2}] * [\text{s}^{-1}]} \left([-] - \text{EXP}([\text{s}^{-1}] * [\text{s}]\right) +$$

$$\frac{\dfrac{[\text{Bq g}^{-1}\text{(wet weight)}]}{[\text{Bq g}^{-1}\text{(dry weight)}]} * [\text{Bq m}^{-3}]}{[\text{g(dry weight) m}^{-3}]} = [\text{Bq g}^{-1}\text{(wet weight)}]$$

Note 1: In DRYRHO equation the factor of 1000 $[\text{g kg}^{-1}]$ is a conversion factor.

Note 2: For AIRC(nuc,loc):
loc = 1 to 80 for v=1 and v=2
81 (total study area average) for v=3 and v=5
82 (watershed area) for v=4

Note 3: CVEG(nuc,(v=1,2,3,4,5),loc) are defined, respectively, as AVEGC, BVEGC, SUFOC, BRWSC and LICHC in Chapter 8 of SENES Vol. 3. SPTC(nuc,(v=1,2,3,4,5)) are defined in Chapter 8 of SENES Vol. 3 as SPTCAV, SPTCBV, SPTCSF, SPTCF and SPTCL (SENES letter 1986-12-02), respectively. CVEG and SPTC have been used in Figure 2.6 in the interests of clarity.

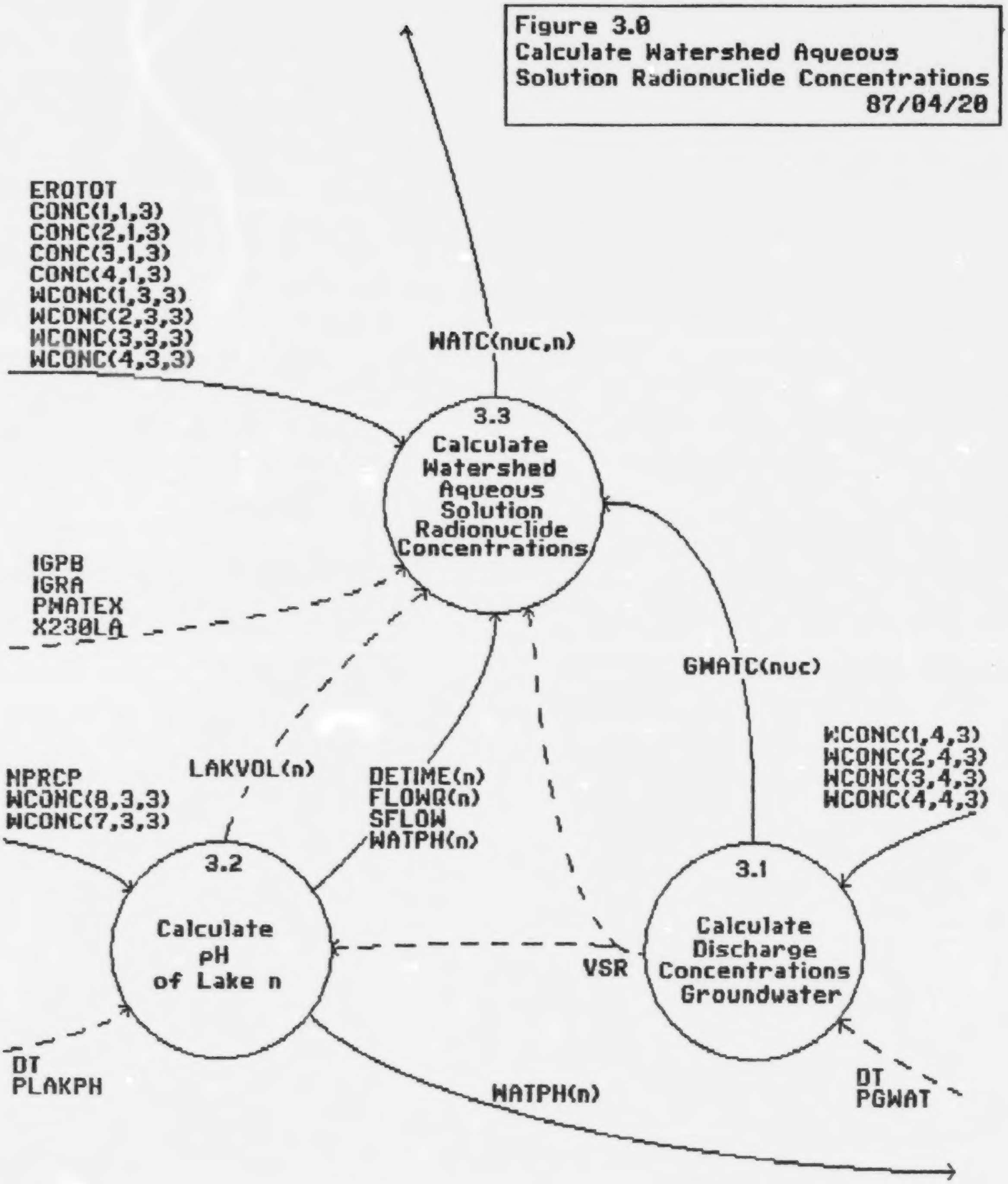


Figure 3.0
Calculate Watershed Aqueous
Solution Radionuclide Concentrations
87/04/20

EROTOT
CONC(1,1,3)
CONC(2,1,3)
CONC(3,1,3)
CONC(4,1,3)
WCONC(1,3,3)
WCONC(2,3,3)
WCONC(3,3,3)
WCONC(4,3,3)
WATC(nuc,n)
3.3
Calculate Watershed Aqueous Solution Radionuclide Concentrations
IGPB
IGRA
PWATEX
X230LA
GWATC(nuc)
WCONC(1,4,3)
WCONC(2,4,3)
WCONC(3,4,3)
WCONC(4,4,3)
NPRCP
WCONC(8,3,3)
WCONC(7,3,3)
LAKVOL(n)
DETIME(n)
FLOWQ(n)
SFLOW
WATPH(n)
3.2
Calculate pH of Lake n
3.1
Calculate Discharge Concentrations Groundwater
VSR
DT
PLAKPH
WATPH(n)
DT
PGWAT

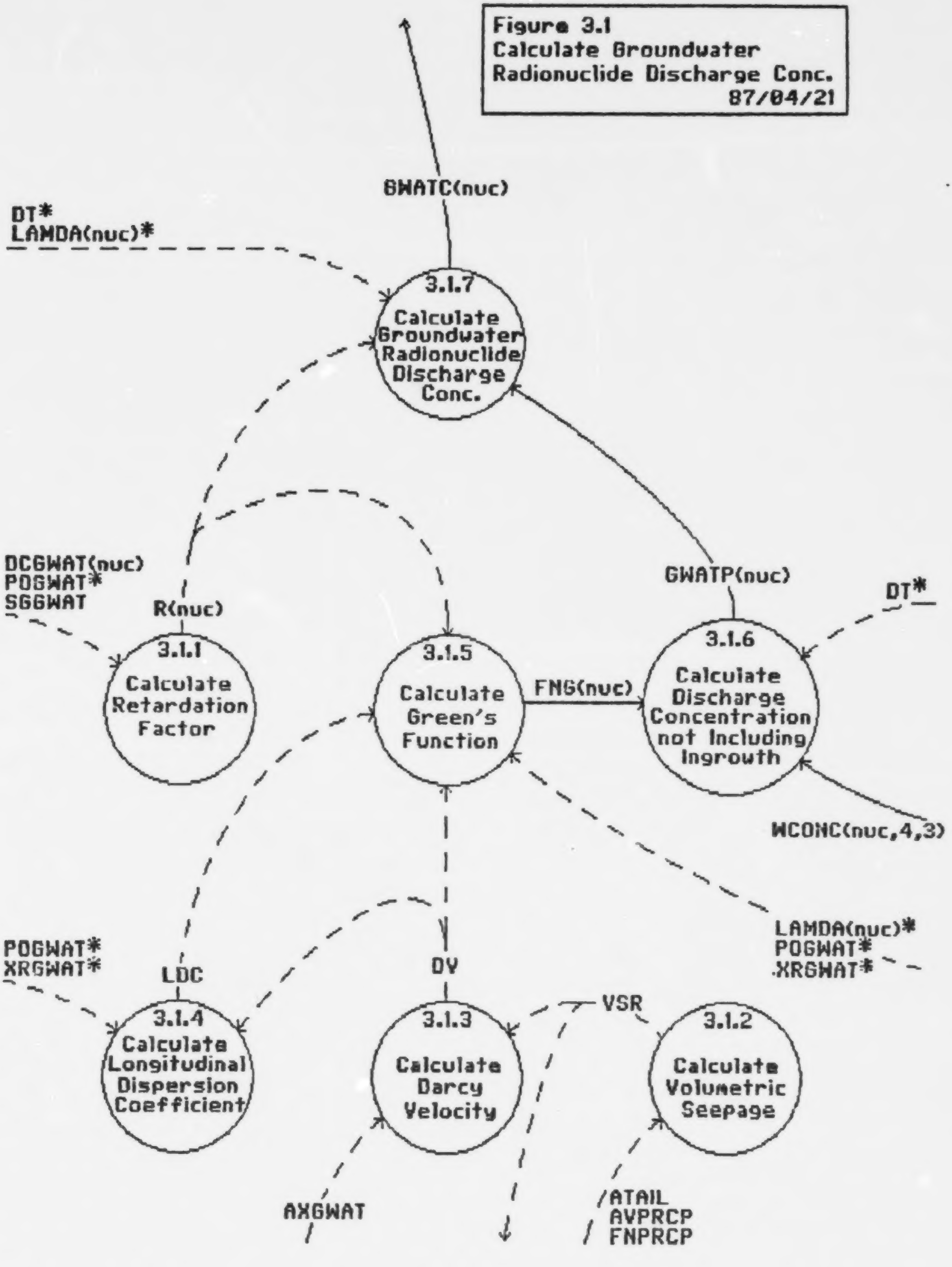


Figure 3.1
Calculate Groundwater
Radionuclide Discharge Conc.
87/04/21

GWATC(nuc)
DT*
LAMDA(nuc)*
3.1.7
Calculate Groundwater Radionuclide Discharge Conc.
DCGWAT(nuc)
POGWAT*
SGGWAT
R(nuc)
3.1.1
Calculate Retardation Factor
3.1.5
Calculate Green's Function
FNG(nuc)
GWATP(nuc)
DT*
3.1.6
Calculate Discharge Concentration not Including Ingrowth
WCONC(nuc,4,3)
LAMDA(nuc)*
POGWAT*
XRGWAT*
POGWAT*
XRGWAT*
LDC
DV
VSR
3.1.4
Calculate Longitudinal Dispersion Coefficient
3.1.3
Calculate Darcy Velocity
3.1.2
Calculate Volumetric Seepage
AXGWAT
ATAIL
AVPRCP
FNPRCP

R(nuc) - RETARDATION FACTOR [-]. A bulk retardation factor for a particular element (Pb, Ra, U, Th).

Figure 3.1.1
Calculate RETARDATION FACTOR
(R(nuc))

SGGWAT
DCGWAT - - -> R(nuc)
POGWAT

Short Name	Long Name	SI Unit	Source
DCGWAT(nuc)	DISTRIBUTION COEFFICIENT FOR RADIONUCLIDE	$[m^3\ kg^{-1}]$	Sampled
POGWAT	AQUIFER POROSITY	[-]	Sampled
R(nuc)	RETARDATION FACTOR	[-]	3.1.1
SGGWAT	SAND SOIL DENSITY	$[kg\ m^{-3}]$	Sampled

R = 1 + SGGWAT * DCGWAT * (1-POGWAT) / POGWAT (eqn. 9.5; see Note 1)

Unit check:

$[-] + [kg\ m^{-3}] * [m^3\ kg^{-1}] * ([-] - [-]) = [-]$

Note 1: SENES ρ_b was defined as $\rho_b = \rho_s$ (1-n) in a letter (1986-11-04). This was combined with equation (9.5) to derive the equation used above.

Note 2: The values "1" have been assumed to be dimensionless.

Figure 3.1.2
Calculate VOLUMETRIC
SEEPAGE
(VSR)

VSR - VOLUMETRIC SEEPAGE [m^3 a^{-1}]. Volumetric seepage rate through the aquifer assumed equal to the average tailings seepage rate.

$$\begin{tikzcd}\begin{matrix}\text{FNPRCP}\\ \text{AVPRCP}\\ \text{ATAIL}\end{matrix} \arrow[r, dashed] & \text{VSR}\end{tikzcd}$$

Short Name	Long Name	SI Unit	Source
ATAIL	INITIAL EXPOSED TAILINGS SURFACE AREA	[m^2]	Sampled
AVPRCP	AVERAGE NET PRECIPITATION	[m a^{-1}]	Sampled
FNPRCP	FRACT. NET PRECIP.	[-]	Sampled
VSR	VOLUMETRIC SEEPAGE	[m^3 a^{-1}]	3.1.2

$$VSR = FNPRCP * AVPRCP * ATAIL \qquad \text{(eqn. 9.3)}$$

Unit check:

$$[-] * [m\ a^{-1}] * [m^2] = [m^3\ a^{-1}]$$

Figure 3.1.3
Calculate DARCY
VELOCITY
(DV)

DV - DARCY VELOCITY [m a^{-1}]. The Darcy velocity of the groundwater through the aquifer.

$$\begin{array}{l} \text{AXGWAT} \\ \text{VSR} \end{array} \dashrightarrow \text{DV}$$

Short Name	Long Name	SI Unit	Source
AXGWAT	CROSS-SECTIONAL AREA OF FLOW	[m^2]	Sampled
DV	DARCY VELOCITY	[m a^{-1}]	3.1.3
VSR	VOLUMETRIC SEEPAGE	[m^3 a^{-1}]	3.1.2

$$DV = VSR / AXGWAT \qquad \text{(eqn. 9.2)}$$

Unit check:

$$[m^3\ a^{-1}] / [m^2] = [m\ a^{-1}]$$

LDC - LONGITUDINAL DISPERSION COEFFICIENT [m^2 a^{-1}].
The longitudinal dispersion coefficient.

Figure 3.1.4
Calculate LONGITUDINAL
DISPERSION COEFFICIENT
(LDC)

ALDIS
DV - - -> LDC
POGWAT

XRGWAT - - -> ALDIS

Short Name	Long Name	SI Unit	Source
ALDIS	LONGITUDINAL DISPERSIVITY	[m]	(3.1.4)
DV	DARCY VELOCITY	[m a^{-1}]	3.1.3
LDC	LONGITUDINAL DISPERSION COEFFICIENT	[m^2 a^{-1}]	3.1.4
POGWAT	AQUIFER POROSITY	[-]	Sampled
XRGWAT	DISCHARGE DISTANCE	[m]	Sampled

ALDIS = 0.12 * XRGWAT (eqn. 9.19)

LDC = DV * ALDIS / POGWAT (eqn. 9.4)

Unit check:

ALDIS: [-] * [m] = [m]

LDC: [m a^{-1}] * [m] / [-] = [m^2 a^{-1}]

Note: 0.12 in equation (9.19) of SENES Vol. 3 is assumed to be dimensionless.

Figure 3.1.5
Calculate GREEN'S FUNCTION
(FNG(nuc))
(Page 1 of 2)

FNG(nuc) - GREEN'S FUNCTION [-]. The Green's function needed for the calculation of the time dependent radionuclide concentrations in groundwater (nuc= nat-U, tot-Th, Ra-226, Pb-210).

POGWAT
LAMDA(nuc)
R(nuc)
BGW(nuc) - - -> FNG(nuc)
DV
LDC
XRGWAT

POGWAT
R(nuc)
LAMDA(nuc) - - -> BGW(nuc)
DV
LDC

Short Name	Long Name	SI Unit	Source
BGW(nuc)	B PARAMETER	$[m^{-1}]$	(3.1.5)
DV	DARCY VELOCITY	$[m\ a^{-1}]$	3.1.3
FNG(nuc)	GREEN'S FUNCTION	[-]	3.1.5
LAMDA(nuc)	NUCLIDE DECAY CONSTANT	$[a^{-1}]$	Sampled
LDC	LONGITUDINAL DISPERSION COEFFICIENT	$[m^2\ a^{-1}]$	3.1.4
POGWAT	AQUIFER POROSITY	[-]	Sampled
R(nuc)	RETARDATION FACTOR	[-]	3.1.1
XRGWAT	DISCHARGE DISTANCE	[m]	Sampled

$$\mathrm{BGW(nuc)} = \sqrt{\left(\frac{\mathrm{DV}}{2 * \mathrm{POGWAT} * \mathrm{LDC}}\right)^2 + \frac{\mathrm{LAMDA(nuc)} * \mathrm{R(nuc)}}{\mathrm{LDC}}}$$

(eqn. below eqn. 9.12)

$$\mathrm{FNG(nuc)} = \frac{1}{2} * \mathrm{EXP}\left[\frac{\mathrm{DV} * \mathrm{XRGWAT}}{2.0 * \mathrm{POGWAT} * \mathrm{LDC}}\right] * \Big\{\mathrm{EXP}(-\mathrm{XRGWAT} * \mathrm{BGW(nuc)}) *$$

$$\mathrm{ERFC}\left(\frac{\mathrm{XRGWAT} - [(\mathrm{DV}/(\mathrm{POGWAT}*\mathrm{R(nuc)}))^2 + (4*\mathrm{LAMDA(nuc)}*\mathrm{LDC}/\mathrm{R(nuc)})]^{0.5} * \mathrm{TIME}}{2. * (\mathrm{LDC} * \mathrm{TIME}/\mathrm{R(nuc)})^{0.5}}\right)$$

$$+ \mathrm{EXP}(+\mathrm{XRGWAT} * \mathrm{BGW(nuc)}) *$$

$$\mathrm{ERFC}\left(\frac{\mathrm{XRGWAT} + [(\mathrm{DV}/(\mathrm{POGWAT}*\mathrm{R(nuc)}))^2 + (4*\mathrm{LAMDA(nuc)}*\mathrm{LDC}/\mathrm{R(nuc)})]^{0.5} * \mathrm{TIME}}{2 * (\mathrm{LDC} * \mathrm{TIME}/\mathrm{R(nuc)})^{0.5}}\right)\Big\}$$

(part of eqn. 9.12; see Note 3)

Unit check:

$$\mathrm{BGW:}\quad \left\{\left([m\ a^{-1}] / ([-] * [-] * [m^2\ a^{-1}])\right)^2 + [a^{-1}] * [-] / [m^2\ a^{-1}]\right\}^{0.5} = [m^{-1}]$$

Figure 3.1.5
Calculate GREEN'S
FUNCTION
(FNG(nuc))
(Page 2 of 2)

$$\mathrm{FNG} = [-] * \mathrm{EXP}\left(\frac{[\mathrm{m\ a^{-1}}] * [\mathrm{m}]}{[-] * [\mathrm{m^2\ a^{-1}}]}\right) * \left\{\mathrm{EXP}(-[\mathrm{m}] * [\mathrm{m^{-1}}]) *\right.$$

$$\mathrm{ERFC}\left(\frac{[\mathrm{m}] - \left[\left(\frac{[\mathrm{m\ a^{-1}}]}{[-] * [-]}\right)^2 + [-] * [\mathrm{a^{-1}}] * [\mathrm{m^2\ a^{-1}}]\right]^{0.5} * [\mathrm{a}]}{[-] * ([\mathrm{m^2\ a^{-1}}] * [\mathrm{a}] / [-])^{0.5}}\right)$$

$$\left. + \mathrm{EXP(as\ before)} * \mathrm{ERFC}\left[\mathrm{as\ before}\right]\right\} = [-]$$

Note 1: FNG(nuc) is part of SENES eqn. (9.12) as defined by rearranging SENES eqn. (9.13) as $G(x,t) = C(x,t)/C_o$.

Note 2: Factors "2", "4", "½" and "0.5" are assumed to be dimensionless.

Note 3: Inspection of the UTAP2 code shows that:
(a) FNG(nuc) = 0 for t=0. This result also follows from a calculation of ERFC(∞) at t=0.
(b) FNG(nuc) is reset to 0 if the calculated value is less than 1.0E-30.
(BWG, 87-04-09)

GWATP(nuc) - DISCHARGE CONCENTRATION NOT INCLUDING IN-GROWTH [Bq m^{-3}]. The radionuclide concentration at a particular time at the discharge from the aquifer. Does not include in-growth of Pb-210 from Ra-226.

Figure 3.1.6
Calculate DISCHARGE
CONCENTRATION NOT
INCLUDING IN-GROWTH
(GWATP(nuc))

DT≡Δt - - -> GWATP(nuc) <—— WCONC(nuc,4,3)
FNG(nuc)

Short Name	Long Name	SI Unit	Source
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
FNG(nuc)	GREEN'S FUNCTION	[-]	3.1.5
GWATP(nuc)	DISCHARGE CONCENTRATION NOT INCLUDING	[Bq m^{-3}]	3.1.6
WCONC(nuc,4,3)	AQ. RADIONUCLIDE IN BOTTOM SAT. ZONE	[Bq m^{-3}]	1.2.6, 1.3.2.8, 1.4.4.8, 1.5.3.8

at TIME = t ≡ t_k where $t \geq 0$

(The values of TIME, WCONC(nuc,4,3) and FNG(nuc), for all previous steps are required)

(eqn. 9.15 with t_o ≡ TIME=0)

$$\mathrm{GWATP}(\mathrm{nuc},t_k) = \mathrm{WCONC}(\mathrm{nuc},4,3)_{t=0} * \mathrm{FNG}(\mathrm{nuc})_{t=t_k}$$

$$+ \sum_{n=1}^{k-1} \left[\left(\mathrm{WCONC}(\mathrm{nuc},4,3)_{t_n} - \mathrm{WCONC}(\mathrm{nuc},4,3)_{t_{n-1}}\right) * \mathrm{FNG}(\mathrm{nuc})_{(t_k-t_n)}\right]$$

$$+ \left(\mathrm{WCONC}(\mathrm{nuc},4,3)_{t_k} - \mathrm{WCONC}(\mathrm{nuc},4,3)_{t_{k-1}}\right) * \mathrm{FNG}(\mathrm{nuc})_{(t_k-t_{k-1})} / 2.0$$

Unit check: [Bq m^{-3}] * [-] = [Bq m^{-3}] applied to each term

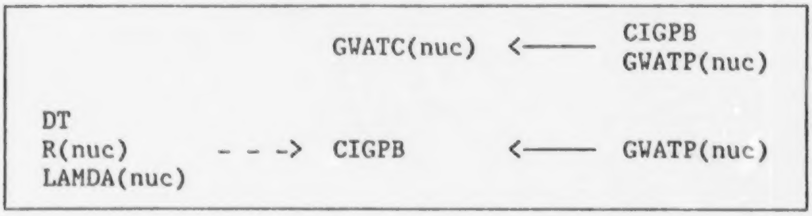
Note 1: This equation approximates the time-variant source as the sum of a series of time independent sources. Equation (9.15) in SENES Vol. 3 is actually more general than the equation given here as there is no need to assume a constant time-step interval. However, normally a constant interval, DT, will be used.

Note 2: An equation of this form is needed for each radionuclide.

Note 3: Solution concentrations are assumed to be zero at t=0 (SENES letter 1987-02-03) and are not defined at t=-Δt.

Figure 3.1.7
Calculate GROUNDWATER RADIONUCLIDE DISCHARGE CONC. (GWATC(nuc))

GWATC(nuc) - GROUNDWATER RADIONUCLIDE DISCHARGE CONC. [Bq m^{-3}]. The radionuclide concentration at the discharge from the aquifer (nuc= nat-U, tot-Th, Ra-226, Pb-210).



Short Name	Long Name	SI Unit	Source
CIGPB	CONCENTRATION PB-210 GROWN-IN FROM RA-226	[Bq m^{-3}]	(3.1.7)
DT	TIME STEP-SIZE	[a]	Sampled
GWATC(nuc)	GROUNDWATER RADIONUCLIDE DISCHARGE CONC.	[Bq m^{-3}]	3.1.7
GWATP(nuc)	DISCHARGE CONCENTRATION NOT INCLUDING IN-GROWTH	[Bq m^{-3}]	3.1.6
LAMDA(nuc)	NUCLIDE DECAY CONSTANT	[a^{-1}]	Sampled
R(nuc)	RETARDATION FACTOR	[-]	3.1.1

If nuc = Pb then:
CIGPB = GWATP(Ra) * (1 - EXP(-LAMDA(PB) * TIME)) * R(RA)/R(PB)
(eqn. 9.8a & 9.8B; see Note 3)

(a) nuc ≠ Pb GWATC(nuc) = GWATP(nuc)
(b) nuc = Pb GWATC(nuc) = GWATP(nuc) + CIGPB (see Note 2)

Unit check:

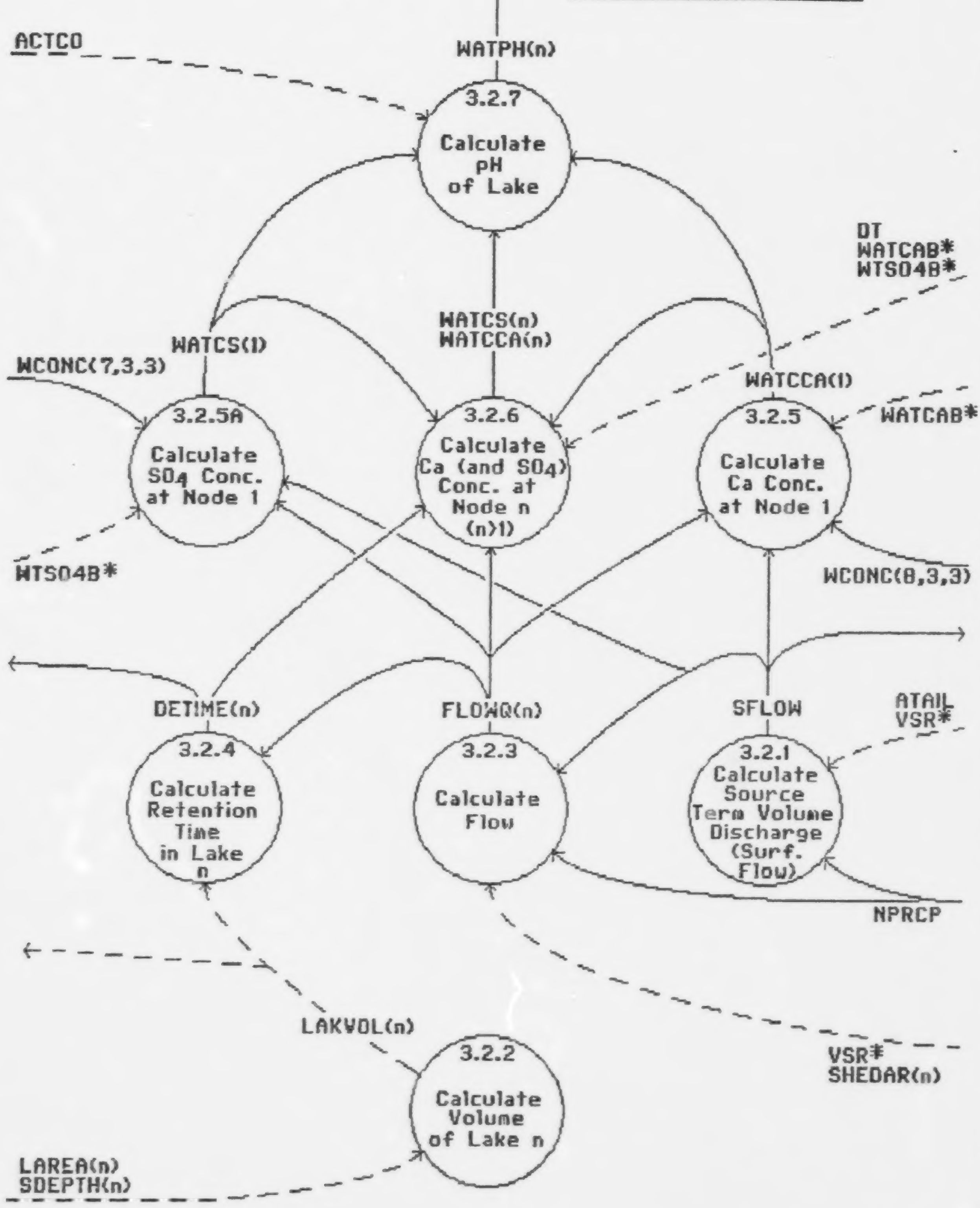
CIGPB: EXP: [a^{-1}] * [a] - [-]
[Bq m^{-3}] * [-] * [-] / [-] = [Bq m^{-3}]
GWATC: [Bq m^{-3}] + [Bq m^{-3}] = [Bq m^{-3}]

Note 1: TIME t is in [a].

Note 2: Inspection of the UTAP2 code shows that GWATC(nuc) = 0 at t=0. (BWG, 87-04-09)

Note 3: Inspection of the UTAP2 code shows that DT is used in the calculation of CIGPB, and not TIME. SYVAC3-UT2 has been changed accordingly. (BWG, 87-05-13)

Figure 3.2
Calculate pH of Lake n
87/04/21


ACTCO
WATPH(n)
3.2.7
Calculate pH of Lake
DT
WATCAB*
WTSO4B*
WATCS(1)
WATCS(n)
WATCCA(n)
WCONC(7,3,3)
WATCCA(1)
WATCAB*
3.2.5A
Calculate SO4 Conc. at Node 1
3.2.6
Calculate Ca (and SO4) Conc. at Node n (n)1)
3.2.5
Calculate Ca Conc. at Node 1
WTSO4B*
WCONC(8,3,3)
DETIME(n)
FLOWQ(n)
SFLOW
ATAIL
VSR*
3.2.4
Calculate Retention Time in Lake n
3.2.3
Calculate Flow
3.2.1
Calculate Source Term Volume Discharge (Surf. Flow)
NPRCP
LAKVOL(n)
VSR*
SHEDAR(n)
3.2.2
Calculate Volume of Lake n
LAREA(n)
SDEPTH(n)

SFLOW - SOURCE TERM VOLUME DISCHARGE (SURF. FLOW) [$m^3\ a^{-1}$]. Volume of source term discharge from the reference tailings area.

Figure 3.2.1
Calculate SOURCE TERM VOLUME DISCHARGE (SURF. FLOW) (SFLOW)

ATAIL
VSR - - -> SFLOW <—— NPRCP

Short Name	Long Name	SI Unit	Source
ATAIL	INITIAL EXPOSED TAILINGS SURFACE AREA	[m^2]	Sampled
NPRCP	NET PRECIPITATION	[$m\ a^{-1}$]	Sampled
SFLOW	SOURCE TERM VOLUME DISCHARGE (SURF. FLOW)	[$m^3\ a^{-1}$]	3.2.1
VSR	VOLUMETRIC SEEPAGE	[$m^3\ a^{-1}$]	3.1.2

$$SFLOW = ATAIL * NPRCP - VSR \qquad \text{(see Note)}$$

Unit check:

$$[m^2] * [m\ a^{-1}] - [m^3\ a^{-1}] = [m^3\ a^{-1}]$$

Note: Equation supplied by SENES (letter 1986-10-15).

Figure 3.2.2
Calculate VOLUME OF LAKE n
(LAKVOL(n))

LAKVOL(n) - VOLUME OF LAKE n [m³]. Volume of the lake in the watershed between nodes (n-1) and n.

LAREA(n)
SDEPTH(n) - - -> LAKVOL(n)

Short Name	Long Name	SI Unit	Source
LAKVOL(n)	VOLUME OF LAKE n	$[m^3]$	3.7.2
LAREA(n)	AREA OF LAKE n	$[m^2]$	Sampled
SDEPTH(n)	DEPTH LAKE n	[m]	Sampled

LAKVOL(n) = LAREA(n) * SDEPTH(n) (pg. 10-27)

Unit check:

$[m^2] * [m] = [m^3]$

FLOWQ(n) - FLOW AT NODE n [m^3 a^{-1}]. Annual volume of surface water flow at node n.

Figure 3.2.3
Calculate FLOW AT
NODE n
(FLOWQ(n))

SHEDAR(n) - - -> FLOWQ(n) <—— NPRCP
VSR SFLOW

Short Name	Long Name	SI Unit	Source
FLOWQ(n)	FLOW AT NODE n	[m^3 a^{-1}]	3.2.3
NPRCP	NET PRECIPITATION	[m a^{-1}]	Sampled
SFLOW	SOURCE TERM VOLUME DISCHARGE (SURF. FLOW)	[m^3 a^{-1}]	3.2.1
SHEDAR(n)	CUM. WATERSHED AREA	[m^2]	Sampled
VSR	VOLUMETRIC SEEPAGE	[m^3 a^{-1}]	3.1.2

$$FLOWQ(n) = SHEDAR(n) * NPRCP + SFLOW + VSR \qquad \text{(eqn. 10.1)}$$

Unit check:

FLOWQ $[m^2] * [m\ a^{-1}] + [m^3\ a^{-1}] + [m^3\ a^{-1}] = [m^3\ a^{-1}]$

Figure 3.2.4
Calculate RETENTION
TIME IN LAKE n
(DETIME(n))

DETIME(n) - RETENTION TIME IN LAKE n [a].
Retention time (or travel time) in
a lake between node (n-1) and node n.

LAKVOL(n) - - -> DETIME(n) <—— FLOWQ(n)

Short Name	Long Name	SI Unit	Source
DETIME(n)	RETENTION TIME IN LAKE n	[a]	3.2.4
FLOWQ(n)	FLOW AT NODE n	[m^3 a^{-1}]	3.2.3
LAKVOL(n)	VOLUME OF LAKE n	[m^3]	3.2.2

DETIME(n) = LAKVOL(n) / FLOWQ(n) (near eqn. 10.29)

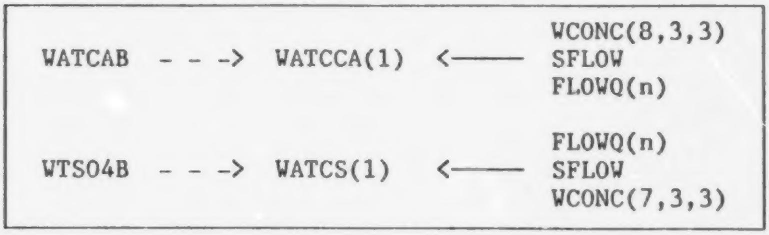
Unit check:

$$[m^3] / [m^3\ a^{-1}] = [a]$$

Figure 3.2.5
Calculate CA CONC. AT NODE 1
(WATCCA(1))
and
Figure 3.2.5A
Calculate SO_4 CONC. AT NODE 1
(WATCS(1))

WATCCA(1) - CA CONCENTRATION AT NODE 1 [mol m^{-3}]. Concentration of calcium in the aqueous phase at node 1 in the watershed.

WATCS(1) - SO_4 CONCENTRATION AT NODE 1 [mol m^{-3}]. Concentration of sulphate in the aqueous phase at node 1 in the watershed.



Short Name	Long Name	SI Unit	Source
FLOWQ(n)	FLOW AT NODE n	[m^3 a^{-1}]	3.2.3
SFLOW	SOURCE TERM VOLUME DISCHARGE (SURFACE FLOW)	[m^3 a^{-1}]	3.2.1
WATCAB	BACKGROUND CALCIUM CONCENTRATION	[mol m^{-3}]	Sampled
WATCCA(1)	CA CONCENTRATION AT NODE 1	[mol m^{-3}]	3.2.5
WATCS(1)	SO_4 CONCENTRATION FOR NODE 1	[mol m^{-3}]	3.2.5A
WCONC(7,3,3)	CONC. OF SO_4 AQ. IN MIXING LAYER	[mol m^{-3}]	1.1.4.6
WCONC(8,3,3)	CONC. OF CA AQ. IN MIXING LAYER	[mol m^{-3}]	1.1.4.7
WTSO4B	BACKGROUND SULPHATE LEVEL	[mol m^{-3}]	Sampled

$$\mathrm{WATCCA(1)} = \frac{\mathrm{SFLOW} * \mathrm{WCONC(8,3,3)} + \mathrm{WATCAB} * (\mathrm{FLOWQ(1)} - \mathrm{SFLOW})}{\mathrm{FLOWQ(1)}}$$

$$\mathrm{WATCS(1)} = \frac{\mathrm{SFLOW} * \mathrm{WCONC(7,3,3)} + \mathrm{WTSO4B} * (\mathrm{FLOWQ(1)} - \mathrm{SFLOW})}{\mathrm{FLOWQ(1)}}$$

(see Note 2)

Unit check: WATCCA(1) and WATCS(1)

$$\frac{[m^3\ a^{-1}]*[mol\ m^{-3}] + [mol\ m^{-3}]*([m^3\ a^{-1}]-[m^3\ a^{-1}])}{[m^3\ a^{-1}]} = [mol\ m^{-3}]$$

Note 1: Form of the equation from SENES letter 1987-02-03.

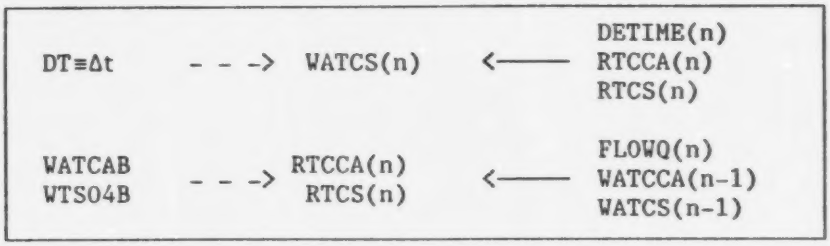
Note 2: Inspection of the UTAP2 code shows that the second occurrence of SFLOW, for both WATCCA(1) and WATCS(1), is not used. This is in disagreement with response #95 in the SENES letter dated 1987-02-03 (see Note 1). We have also deleted it from SYVAC3-UT2. (BWG, 87-04-09)

Figure 3.2.6
Calculate CA (AND SO_4)
CONC. AT NODE n (n>1)

(WATCCA(n) and WATCS(n))
(Page 1 of 2)

WATCCA(n) - CA CONCENTRATION AT NODE N [mol m^{-3}]. Concentration of calcium in the aqueous phase at node n in the watershed (n>1).

WATCS(n) - SO_4 CONCENTRATION AT NODE N [mol m^{-3}]. Concentration of sulphate in the aqueous phase at node n in the watershed (n>1).



Short Name	Long Name	SI Unit	Source
DETIME(n)	RETENTION TIME IN LAKE n	[a]	3.2.4
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
FLOWQ(n)	FLOW AT NODE n	[m^3 a^{-1}]	3.2.3
RTCCA(n)	CA CONCENTRATION PARAMETERS FOR NODE n	[mol m^{-3}]	(3.2.6)
RTCS(n)	SO_4 CONCENTRATION PARAMETERS FOR NODE n	[mol m^{-3}]	(3.2.6)
WATCAB	BACKGROUND CALCIUM LEVEL	[mol m^{-3}]	Sampled
WATCCA(n)	CA CONCENTRATION AT NODE n	[mol m^{-3}]	3.2.6
WATCCA(n-1)	CA CONCENTRATION AT NODE n-1	[mol m^{-3}]	3.2.6, 3.2.5
WATCS(n)	SO_4 CONCENTRATION AT NODE n	[mol m^{-3}]	3.2.6
WATCS(n-1)	SO_4 CONCENTRATION AT NODE n-1	[mol m^{-3}]	3.2.6, 3.2.5A
WTSO4B	BACKGROUND SULPHATE LEVEL	[mol m^{-3}]	Sampled

(a) $$\text{RTCCA(n)} = \frac{\text{FLOWQ(n-1)} * \text{WATCCA(n-1)} + (\text{FLOWQ(n)} - \text{FLOWQ(n-1)}) * \text{WATCAB}}{\text{FLOWQ(n)}}$$

(see Note 1)

(i) if DETIME(n) > 0
Solve the following finite difference equation for WATCCA(n,t)

$$\text{WATCCA(n,t)} = \text{RTCCA(n)} + \left\{\text{WATCCA}(n,t-\Delta t) - \text{RTCCA(n)}\right\} * \text{EXP}\left(\frac{-\text{DT}}{\text{DETIME(n)}}\right)$$

(eqn. 10.5;
see Note 2)

(ii) if DETIME(n) = 0 WATCCA(n) = RTCCA(n)

(b) $$\text{RTCS(n)} = \frac{\text{FLOWQ(n-1)} * \text{WATCS(n-1)} + (\text{FLOWQ(n)} - \text{FLOWQ(n-1)}) * \text{WTSO4B}}{\text{FLOWQ(n)}}$$

(see Note 1)

(i) if DETIME(n) > 0
Solve the following finite difference equation for WATCS(n,t)

$$\text{WATCS(n,t)} = \text{RTCS(n)} + \left\{\text{WATCS}(n,t-\Delta t) - \text{RTCS(n)}\right\} * \text{EXP}\left(\frac{-\text{DT}}{\text{DETIME(n)}}\right)$$

(eqn. 10.5)

(ii) if DETIME(n) = 0 WATCS(n) = RTCS(n)

Figure 3.2.6
Calculate CA (AND SO_4)
CONC. AT NODE n (n>1)

(WATCCA(n) and WATCS(n))
(Page 2 of 2)

Unit check:

$$\left.\begin{array}{l}\text{RTCCA(n)}\\ \text{RTCS(n)}\end{array}\right\} \Big([\text{m}^3\ \text{a}^{-1}] * [\text{mol m}^{-3}] + [\text{m}^3\ \text{a}^{-1}] * [\text{mol m}^{-3}]\Big) \ / \ [\text{m}^3\ \text{a}^{-1}] = [\text{mol m}^{-3}]$$

$$\left.\begin{array}{l}\text{WATCCA(n)}\\ \text{WATCS(n)}\end{array}\right\} [\text{mol m}^{-3}] + \Big([\text{mol m}^{-3}] - [\text{mol m}^{-3}]\Big) * \text{EXP} \left[\frac{\text{a}}{\text{a}}\right] = [\text{mol m}^{-3}]$$

Note 1: RTCCA and RTCS were calculated from a modified version of equations (10.2) and (10.3) (SENES letters 1986-10-15, 1987-03-02 support these modifications).

Note 2: For river links (ending at nodes 3,5,6,8) DETIME(n) is assumed zero and WATCCA(n) = RTCCA(n)
WATCS(n) = RTCS(n)
as only dilution affects river concentrations (SENES pg. 10-6).

Note 3: Assume that WATCCA(n,t=0) = WATCAB and
WATCS(n,t=0) = WTS04B
as initial conditions. (BWG 87-02)

Note 4: Inspection of the UTAP2 code shows that the conditions for (a) and (b) - (i) and (ii) are actually based on the following logic:
For lake nodes n (as determined by a UTAP2 input for "L" denoting lakes), the exponent in the equations for WATCCA(n) and WATCS(n) is -DT/DETIME if -DT/DETIME $\geq$ -85; otherwise EXP(-DT(DETIME) is set to zero. SYVAC3-UT2 was modified accordingly, using the comparison: if DETIME > 0 followed by if (-DT/DETIME$\geq$ -85) instead of if DETIME > 0. (BWG, 87-04-09)

Figure 3.2.7
Calculate PH OF LAKE (n)
(WATPH(n))

WATPH(n) - PH OF LAKE (n) [-].
pH of lake between nodes (n-1) and n.

ACTCO - - -> WATPH(n) <—— WATCCA(n)
WATCS(n)

Short Name	Long Name	SI Unit	Source
ACTCO	ACTIVITY COEFF. IN LAKE	[-]	Sampled
WATCCA(n)	CA CONCENTRATION AT NODE n	$[\mathrm{mol\ m^{-3}}]$	3.2.5, 3.2.6
WATCS(n)	SO4 CONCENTRATION AT NODE n	$[\mathrm{mol\ m^{-3}}]$	3.2.5A, 3.2.6
WATPH(n)	PH OF LAKE	[-]	3.2.7

Solve the following equation iteratively for pH:

$$3\left[\frac{10^{8.5-3pH}}{(\mathrm{ACTCO})^{9/4}}\right] + 2\left[\frac{10^{3.91-2pH}}{\mathrm{ACTCO}}\right] + \left[10^{0.3-pH}\right] + \left[10^{-3.86}\right] + 2 * 10^{-3} *$$

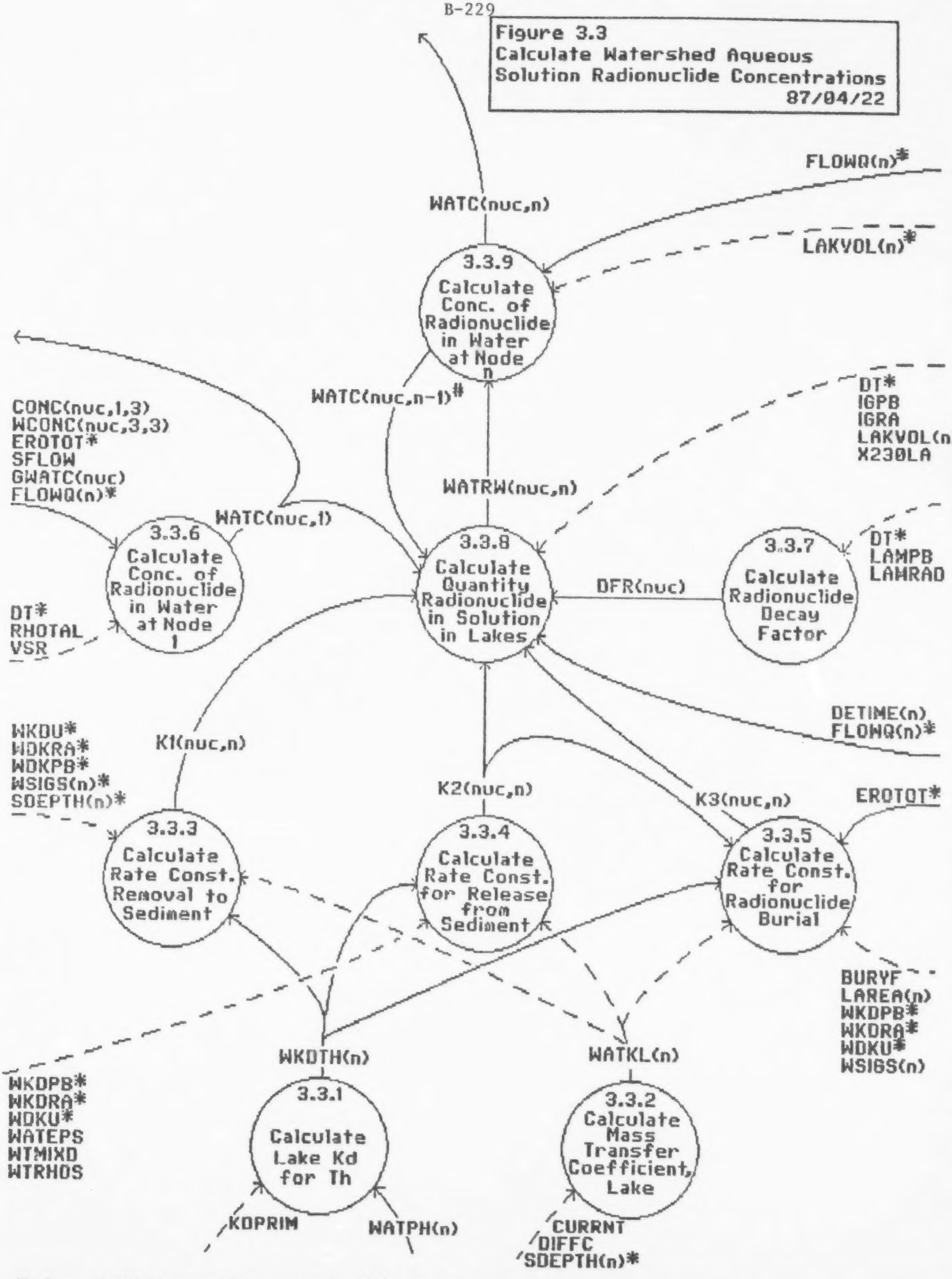
$$\mathrm{WATCCA}(n) = 10^{-3} * \mathrm{WATCS}(n) * \left[\frac{2 - (\mathrm{ACTCO})^{3/4} * 10^{11.7-3pH}}{1 + (\mathrm{ACTCO})^{3/4} * 10^{11.7-3pH}}\right] + \left[\frac{10^{pH-11.0}}{(\mathrm{FACTCO})^{1/4}}\right]$$

(eqn. 10.8)

Note 1: pH is used as an abbreviation for WATPH(n) in the above equation.

Note 2: WATCCA and WATCS must be in units of $[\mathrm{mol\ dm^{-3}}]$ to match the other terms in the above equation. The conversion factor is 10^{-3} $[\mathrm{m^3\ dm^{-3}}]$ and equation (10.8) has been modified to include this factor.

Figure 3.3
Calculate Watershed Aqueous
Solution Radionuclide Concentrations
87/04/22


WATC(nuc,n)
FLOWQ(n)*
LAKVOL(n)*
3.3.9
Calculate Conc. of Radionuclide in Water at Node n
WATC(nuc,n-1)#
DT*
IGPB
IGRA
LAKVOL(n)*
X230LA
CONC(nuc,1,3)
WCONC(nuc,3,3)
EROTOT*
SFLOW
GWATC(nuc)
FLOWQ(n)*
WATRW(nuc,n)
WATC(nuc,1)
3.3.6
Calculate Conc. of Radionuclide in Water at Node 1
DT*
RHOTAL
VSR
3.3.8
Calculate Quantity Radionuclide in Solution in Lakes
DFR(nuc)
3.3.7
Calculate Radionuclide Decay Factor
DT*
LAMPB
LAMRAD
DETIME(n)
FLOWQ(n)*
WKDU*
WDKRA*
WDKPB*
WSIGS(n)*
SDEPTH(n)*
K1(nuc,n)
K2(nuc,n)
K3(nuc,n)
EROTOT*
3.3.3
Calculate Rate Const. Removal to Sediment
3.3.4
Calculate Rate Const. for Release from Sediment
3.3.5
Calculate Rate Const. for Radionuclide Burial
BURYF
LAREA(n)
WKDPB*
WKDRA*
WDKU*
WSIGS(n)
WKDTH(n)
WATKL(n)
WKDPB*
WKDRA*
WDKU*
WATEPS
WTMIXD
WTRHOS
3.3.1
Calculate Lake Kd for Th
3.3.2
Calculate Mass Transfer Coefficient, Lake
KDPRIM
WATPH(n)
CURRNT
DIFFC
SDEPTH(n)*

Note: WATC(nuc,n-1) is required in 3.3.8 and thus the calculation of WATC(nuc,n) must be done node by node for each time step.

WKDTH(n) - LAKE KD FOR TH [$m^3\ g^{-1}$].
Distribution coefficient from water to lake sediment for thorium in the lake between node (n-1) and node n.

Figure 3.3.1
Calculate LAKE KD FOR TH
(WKDTH(n))

$$\boxed{\text{KDPRIM} \dashrightarrow \text{WKDTH(n)} \longleftarrow \text{WATPH(n)}}$$

Short Name	Long Name	SI Unit	Source
KDPRIM	SLOPE TH KD	[$m^3\ g^{-1}$]	Sampled
WATPH(n)	PH OF LAKE (n)	[-]	3.2.7
WKDTH(n)	LAKE KD FOR TH	[$m^3\ g^{-1}$]	3.3.1

If $\text{WATPH(n)} \geq 4$

$$\text{WKDTH(n)} = \text{KDPRIM} * (\text{WATPH(n)} - 4.0) + 2.0 \times 10^{-3}$$

(eqn. 10.13; see Note 1)

If $\text{WATPH(n)} < 4$

$$\text{WKDTH(n)} = 2.0 \times 10^{-3}$$

Unit check: $[m^3\ g^{-1}] * [-] + [m^3\ g^{-1}] = [m^3\ g^{-1}]$

Note: Both KDPRIM and the constant 2.0×10^{-3} in eqn. (10.13) have units of [$m^3\ g^{-1}$]. The units of the latter are assumed from discussion below eqn. (10.13).

Figure 3.3.2
Calculate MASS TRANSFER COEFFICIENT, LAKE (WATKL(n))

WATKL(n) - MASS TRANSFER COEFFICIENT, LAKE [m a^{-1}]. Mass transfer coefficient of the radionuclides into the lake water column from the sediment in the lake between nodes (n-1) and n.

```
CURRNT
DIFFC        - - ->    WATKL(n)
SDEPTH(n)
```

Short Name	Long Name	SI Unit	Source
CURRNT	CURRENT VELOCITY	[m a^{-1}]	Sampled
DIFFC	SEDIMENT DIFFUSIVITY COEFFICIENT	[m^2 a^{-1}]	Sampled
SDEPTH(n)	DEPTH LAKE n	[m]	Sampled
WATKL(n)	MASS TRANSFER COEFFICIENT, LAKE	[m a^{-1}]	3.3.2

(a) If SDEPTH(n) > 0

$$WATKL(n) = \sqrt{\frac{DIFFC * CURRNT}{\pi * SDEPTH(n)}} \qquad [m\ a^{-1}]$$

(eqn. 10.15, 10.16; see also pg. 10-23)

(b) If SDEPTH(n) = 0 WATKL(n) = 0

Unit check:

$$\left([m^2\ a^{-1}] * [m\ a^{-1}] / [m]\right)^{1/2} = [m\ a^{-1}]$$

Note: Condition (b) is not specified by SENES, but is useful in correctly restricting subsequent calculations to lake nodes.

Figure 3.3.3
Calculate RATE CONST.
REMOVAL TO SEDIMENT
(K1(nuc,n))

K1(nuc,n) - RATE CONST. FOR REMOVAL OF RADIONUCLIDE TO SEDIMENT $[a^{-1}]$. Rate constant for removal of radionuclide nuc (nuc = U, Th, Ra, Pb) from the lake water column of the lake between watershed nodes (n-1) and n.

$$\begin{tikzcd}
\begin{array}{l}\text{WSIGS(n)}\\ \text{WKDU}\\ \text{WKDPB}\\ \text{WKDRA}\\ \text{SDEPTH}\\ \text{WATKL(n)}\end{array} \arrow[r, dashed] & \text{K1(nuc,n)} & \text{WKDTH(n)} \arrow[l]
\end{tikzcd}$$

Short Name	Long Name	SI Unit	Source
K1(nuc,n)	RATE CONST. REMOVAL OF RADIONUCLIDE TO SEDIMENT	$[a^{-1}]$	3.3.3
SDEPTH(n)	DEPTH LAKE n	[m]	Sampled
WATKL(n)	MASS TRANSFER COEFFICIENT, LAKE	$[m\ a^{-1}]$	3.3.2
WKDU, WKDPB, & WKDRA	LAKE KD FOR U, PB, RA	$[m^3\ g^{-1}]$	Sampled
WKDTH(n)	LAKE KD FOR TH	$[m^3\ g^{-1}]$	3.3.1
WSIGS(n)	RATE OF SEDIMENTING MATERIAL REMOVAL	$[g\ m^{-2}\ a^{-1}]$	Sampled

If WATKL(n) > 0

$$\text{K1(nuc,n)} = \left\{ \text{WSIGS(n)} * \begin{pmatrix}\text{WKDU}\\ \text{WKDTH(n)}\\ \text{WKDRA}\\ \text{WKDPB}\end{pmatrix} + \text{WATKL(n)} \right\} / \text{SDEPTH(n)} \qquad \text{(eqn. 10.26)}$$

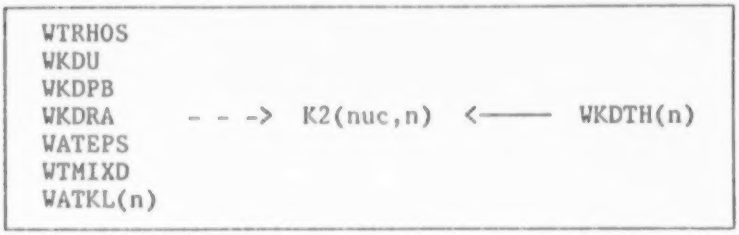
Unit check:

$$([g\ m^{-2}\ a^{-1}] * [m^3\ g^{-1}] + [m\ a^{-1}]) \ /\ [m] = [a^{-1}]$$

Note: In the equation WKDU, WKDTH(n), WKDRA and WKDPB are used, repectively, in the calculation of K1(nuc,n), nuc = U, Th, Ra and Pb.

K2(nuc,n) - RATE CONST. FOR RELEASE OF RADIONUCLIDE FROM SEDIMENT [a^{-1}]. Rate constant for release of radionuclide i (i = U, Th, Ra, Pb) from the lake water column of the lake between watershed nodes (n-1) and n.

Figure 3.3.4
Calculate RATE CONST.
FOR RELEASE FROM
SEDIMENT
(K2(nuc,n))



Short Name	Long Name	SI Unit	Source
K2(nuc,n)	RATE CONST. FOR RELEASE OF RADIONUCLIDE FROM SEDIMENT	[a^{-1}]	3.3.4
WATEPS	SEDIMENT POROSITY	[-]	Sampled
WATKL(n)	MASS TRANSFER COEFFICIENT, LAKE	[$m\ a^{-1}$]	3.3.2
WKDTH(n)	LAKE KD FOR TH	[$m^3\ g^{-1}$]	3.3.1
WKDU, WKDPB & WKDRA	LAKE KD FOR U, PB, RA	[$m^3\ g^{-1}$]	Sampled
WTMIXD	SEDIMENT ZONE THICKNESS	[m]	Sampled
WTRHOS	SEDIMENT SOLID DENSITY	[$g\ m^{-3}$]	Sampled

If WATKL(n) > 0

$$K2(nuc,n) = \frac{1.05 * WATKL(n)}{WTMIXD * \left\{ \begin{pmatrix} WKDU \\ WKDTH(n) \\ WKDRA \\ WKDPB \end{pmatrix} * WTRHOS * (1.0 - WATEPS) + WATEPS \right\}}$$

(eqn. 10.27)

Unit check:

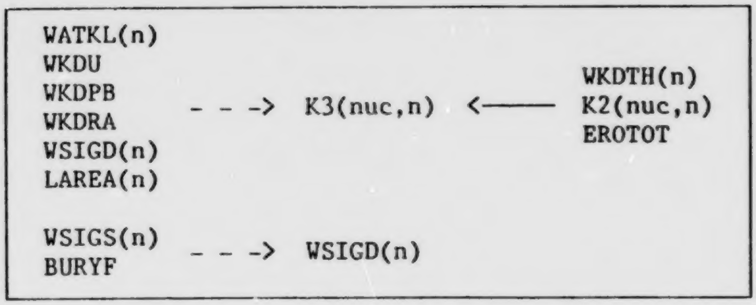
$$[m\ a^{-1}] \;/\; \Big([m] * \{[m^3\ g^{-1}] * [g\ m^{-3}] * [-] + [-]\}\Big) = [a^{-1}]$$

Note 1: 1.05 in the numerator and "1" in the denominator are assumed to be dimensionless.

Note 2: In the equation WKDU, WKDTH(n), WKDRA and WKDPB are used, respectively, in the calculation of K2(nuc,n), nuc = U, Th, Ra, Pb.

Figure 3.3.5
Calculate RATE CONST.
FOR RADIONUCLIDE BURIAL
(K3(nuc,n))

K3(nuc,n) - RATE CONST. FOR RADIONUCLIDE BURIAL $[a^{-1}]$. Rate constant for loss of radionuclide nuc (nuc = U, Th, Ra, Pb) to deep lake sediment of the lake between watershed nodes (n-1) and n.



Short Name	Long Name	SI Unit	Source
BURYF	FRACTION TO DEEP SEDIMENT	[-]	Sampled
EROTOT	EROSION MASS LOSS FROM TAILINGS	[kg]	1.6.3.10
K2(nuc,n)	RATE CONST. FOR RELEASE OF RADIONUCLIDE FROM SEDIMENT	$[a^{-1}]$	3.3.4
K3(nuc,n)	RATE CONST. FOR RADIONUCLIDE BURIAL	$[a^{-1}]$	3.3.5
LAREA(n)	AREA OF LAKE	$[m^2]$	Sampled
WATKL(n)	MASS TRANSFER COEFFICIENT, LAKE	$[m\ a^{-1}]$	3.3.2
WKDTH(n)	LAKE KD FOR TH	$[m^3\ g^{-1}]$	3.3.1
WKDU, WKDPB, WKDRA	LAKE KD FOR U, PB, RA	$[m^3\ g^{-1}]$	Sampled
WSIGD(n)	RATE OF SEDIMENT BURIAL	$[g\ m^{-2}\ a^{-1}]$	(3.3.5)
WSIGS(n)	RATE OF SEDIMENTING MATERIAL REMOVAL	$[g\ m^{-2}\ a^{-1}]$	Sampled

If WATKL(n) > 0

$$\text{WSIGD(n)} = \text{WSIGS(n)} * \text{BURYF} \qquad \text{(eqn. 10.12; see Note 3)}$$

$$\text{K3(nuc,n)} = \text{K2(nuc,n)} * \text{WSIGD(n)} * \begin{Bmatrix} \text{WKDU} \\ \text{WKDTH(n)} \\ \text{WKDRA} \\ \text{WKDPB} \end{Bmatrix} / \text{WATKL(n)}$$

(eqn. 10.27, 10.28)

Unit check:

WSIGD: $[g\ m^{-2}\ a^{-1}] * [-] = [g\ m^{-2}\ a^{-1}]$

K3: $[a^{-1}] * [g\ m^{-2}\ a^{-1}] * [m^3\ g^{-1}] / [m\ a^{-1}] = [a^{-1}]$

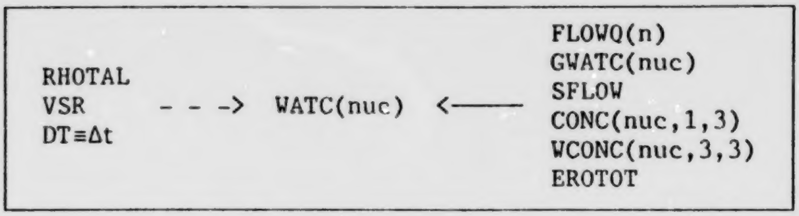
Note 1: In the equation for K3, WKDU, WKDTH(n), WKDRA and WKDPB are used, respectively, in the calculation of K3(nuc,n), nuc = U, Th, Ra, Pb.

Note 2: K2(nuc,n) has been used to modify (simplify) the expression for K3(nuc,n).

Note 3: Inspection of the UTAP2 code shows that, for the first lake (f.l.) in the system,
WSIGD(f.l.) = BURYF * [WSIGS(f.l.) + EROTOT * 1000/DT/LAREA(f.l.)].
In the system studied here, f.l.=2. SYVAC3-UT2 has been modified accordingly. (BWG, 87-04-09)

Figure 3.3.6
Calculate CONC. OF RADIONUCLIDE IN WATER AT NODE 1 (WATC(nuc,1))

WATC(nuc,1) - CONCENTRATION OF RADIONUCLIDE IN WATER AT WATERSHED NODE 1 [Bq m^{-3}]. Concentration of radionuclide (nuc = nat-U, tot-Th, Ra-226, Pb-210) in the aqueous phase at node 1 of the watershed.



Short Name	Long Name	SI Unit	Source
CONC(nuc,1,3)	CONC. SOLID RADIONUCLIDE IN LAYER 1	[Bq m^{-3}]	1.2.3, 1.3.2.5B 1.4.1.4, 1.5.1.3
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
EROTOT	EROSION MASS LOSS FROM TAILINGS	[kg]	1.6.3.10
FLOWQ(n)	FLOW AT NODE n	[m^3 a^{-1}]	3.2.3
GWATC(nuc)	GROUNDWATER RADIONUCLIDE DISCHARGE CONC.	[Bq m^{-3}]	3.1.7
RHOTAL	TAILINGS BULK DENSITY	[g m^{-3}]	Sampled
SFLOW	SOURCE TERM VOLUME DISCHARGE	[m^3 a^{-1}]	3.2.1
VSR	VOLUMETRIC SEEPAGE	[m^3 a^{-1}]	3.1.2
WATC(nuc,1)	CONCENTRATION OF RADIONUCLIDE IN WATER AT WATERSHED NODE 1	[Bq m^{-3}]	3.3.6
WCONC(nuc,3,3)	AQ. RADIONUCLIDE IN MIXING ZONE	[Bq m^{-3}]	1.2.5, 1.3.2.7, 1.4.4.5, 1.5.3.5

For nuc= U, Th, Ra and Pb:

WATC(nuc,1) =

$$\frac{\text{SFLOW} * \text{WCONC(nuc,3,3)} + \text{VSR} * \text{GWATC(nuc)} + \dfrac{10^3 * \text{EROTOT} * \text{CONC(nuc,1,3)}}{\text{DT} * \text{RHOTAL}}}{\text{FLOWQ(1)}}$$

(eqn. 10.9; see Note 1)

Unit check:

$$\frac{[m^3\ a^{-1}] * [Bq\ m^{-3}] + [m^3\ a^{-1}] * [Bq\ m^{-3}] + \dfrac{[g\ kg^{-1}] * [kg] * [Bq\ m^{-3}]}{[a] * [g\ m^{-3}]}}{[m^3\ a^{-1}]} = [Bq\ m^{-3}]$$

Note 1: Equation (10.9) has been modified and verification from SENES obtained (1987-03-02; response #95). There exists an apparent typographical error in the SENES letter (x instead of + before the last term) that has been ignored.

Note 2: The region between the tailings and node 1 is a river.

Note 3: A factor of 10^3 [g kg^{-1}] has been introduced to maintain consistency of units.

Note 4: Inspection of the UTAP2 code shows that the equation referenced in Note 1 is missing brackets; FLOWQ(1) should divide the entire expression as shown above. (BWG, 87-05-05)

Figure 3.3.7
Calculate RADIONUCLIDE DECAY FACTOR (DFR(nuc), nuc = Ra-226, Pb-210)

DFR(nuc) - RADIONUCLIDE DECAY FACTOR [-]. Factor to allow for the decay of radionuclide during the residence time in lake water or lake sediments (nuc = Ra-226, Pb-210).

LAMPB
LAMRAD - - -> DFR(nuc)
DT≡Δt

Short Name	Long Name	SI Unit	Source
DFR(nuc)	RADIONUCLIDE DECAY FACTOR	[-]	3.3.7
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
LAMPB	PB-210 DECAY CONSTANT	[a^{-1}]	Sampled
LAMRAD	RA-226 DECAY CONSTANT	[a^{-1}]	Sampled

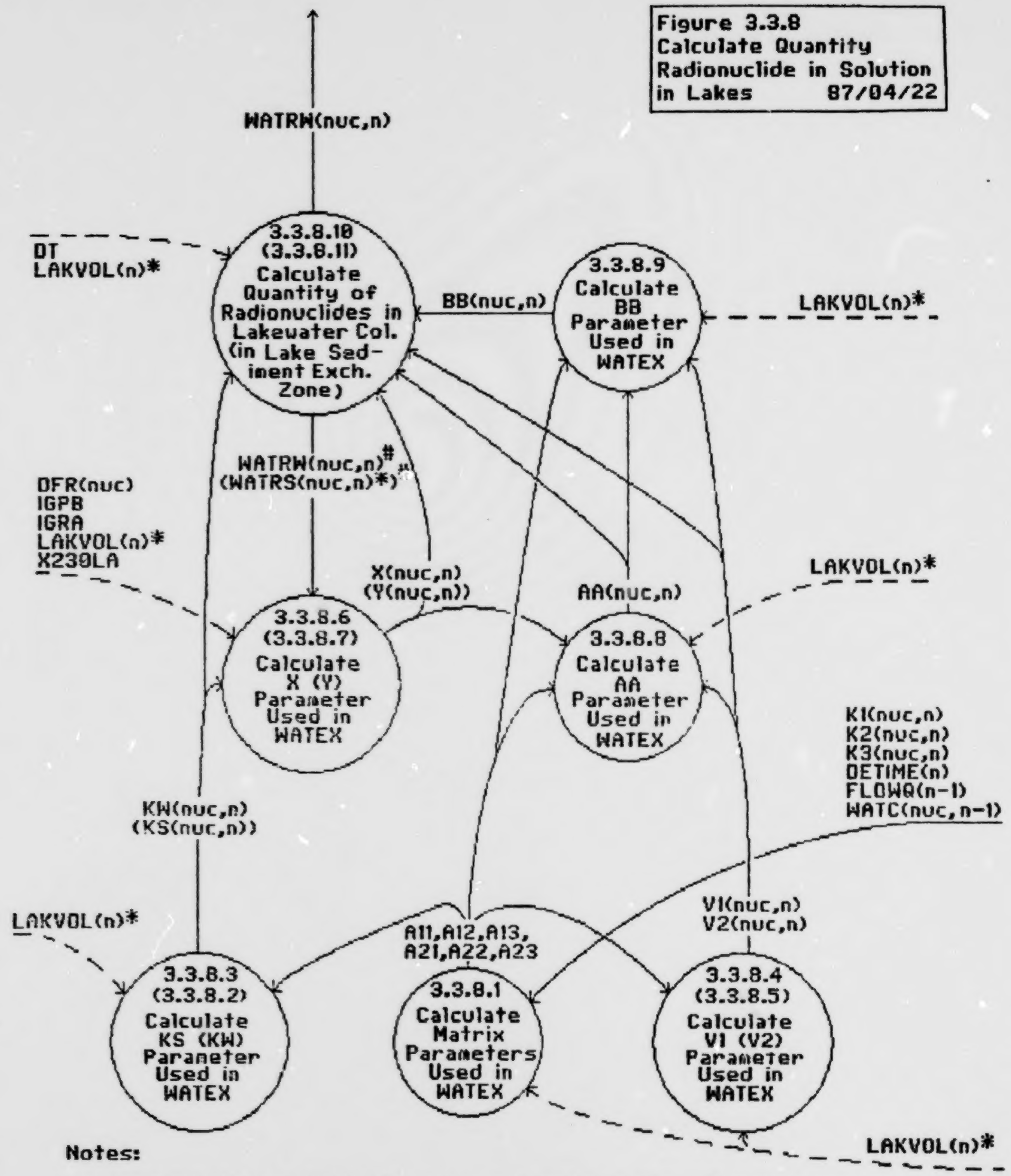
DFR(Pb) = EXP (-LAMPB * DT) (see Note)

DFR(Ra) = EXP (-LAMRAD * DT)

Unit check:
EXP([a^{-1}] * [a]) = [-]

Note: These expressions are portions of equations on page 10-30 of SENES Vol. 3. DFR(Pb) and DFR(Ra) are used to simplify those equations.

Figure 3.3.8
Calculate Quantity
Radionuclide in Solution
in Lakes 87/04/22



WATRW(nuc,n)
DT
LAKVOL(n)*
3.3.8.10
(3.3.8.11)
Calculate Quantity of Radionuclides in Lakewater Col. (in Lake Sediment Exch. Zone)
BB(nuc,n)
3.3.8.9
Calculate BB Parameter Used in WATEX
LAKVOL(n)*
WATRW(nuc,n)#,
(WATRS(nuc,n)*)
DFR(nuc)
IGPB
IGRA
LAKVOL(n)*
X230LA
X(nuc,n)
(Y(nuc,n))
AA(nuc,n)
LAKVOL(n)*
3.3.8.6
(3.3.8.7)
Calculate X (Y) Parameter Used in WATEX
3.3.8.8
Calculate AA Parameter Used in WATEX
K1(nuc,n)
K2(nuc,n)
K3(nuc,n)
DETIME(n)
FLOWQ(n-1)
WATC(nuc,n-1)
KW(nuc,n)
(KS(nuc,n))
V1(nuc,n)
V2(nuc,n)
LAKVOL(n)*
A11,A12,A13,
A21,A22,A23
3.3.8.3
(3.3.8.2)
Calculate KS (KW) Parameter Used in WATEX
3.3.8.1
Calculate Matrix Parameters Used in WATEX
3.3.8.4
(3.3.8.5)
Calculate V1 (V2) Parameter Used in WATEX
LAKVOL(n)*

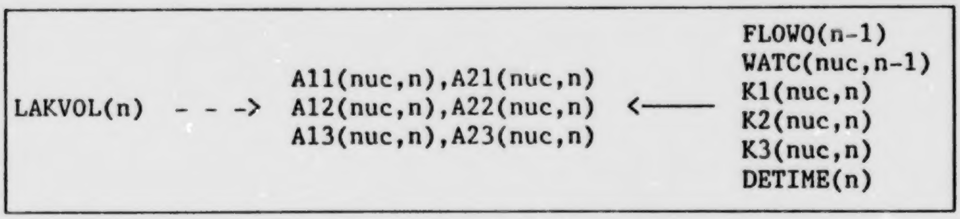
Notes:

1. "#" indicates that the value required is the value from the previous time step.
2. By definition n > 1 because node 1 must be a river node. Therefore the use of the conditions DETIME(n) > 0 or LAKVOL(n) > 0 also define n to be n > 1.
3. The multiply-labelled bubbles have the parallel data flows shown, except that AA(nuc,n) is not required by 3.3.8.11, V2(nuc,n) is not required by 3.3.8.9, and BB(nuc,n) is not required by 3.3.8.10.
4. The variables A11, A12 etc. are functions of nuc and n.

Figure 3.3.8.1
Calculate MATRIX PARAMETERS USED IN WATEX
(A11(nuc,n), A21(nuc,n)
A12(nuc,n), A13(nuc,n)
A22(nuc,n), A23(nuc,n))

A11(nuc,n) [Bq a^{-1}] A21(nuc,n) [Bq a^{-1}]
A12(nuc,n) [a^{-1}] A22(nuc,n) [a^{-1}]
A13(nuc,n) [a^{-1}] A23(nuc,n) [a^{-1}]

MATRIX PARAMETERS USED IN WATEX. Intermediate parameters used in the calculation of WATRW and WATRS in the WATEX module.



Short Name	Long Name	SI Unit	Source
A11(nuc,n)A21(nuc,n)	MATRIX PARAMETERS USED IN WATEX	[Bq a^{-1}]	3.3.8.1
A12(nuc,n)A22(nuc,n) A13(nuc,n)A23(nuc,n)	MATRIX PARAMETERS USED IN WATEX	[a^{-1}]	3.3.8.1
DETIME(n)	RETENTION TIME IN LAKE	[a]	3.2.4
FLOWQ(n-1)	FLOW AT NODE n-1	[m^3 a^{-1}]	3.2.3
K1(nuc,n)	RATE CONST. FOR REMOVAL OF RADIONUCLIDE TO SEDIMENT	[a^{-1}]	3.3.3
K2(nuc,n)	RATE CONST. FOR RELEASE OF RADIONUCLIDE FROM SEDIMENT	[a^{-1}]	3.3.4
K3(nuc,n)	RATE CONST. FOR RADIONUCLIDE BURIAL	[a^{-1}]	3.3.5
LAKVOL(n)	VOLUME OF LAKE n	[m^3]	3.2.2
WATC(nuc,(n-1)	CONCENTRATION OF RADIONUCLIDE IN WATER AT WATERSHED NODE (n-1)	[Bq m^{-3}]	3.3.9, 3.3.6

If LAKVOL(n) > 0

A11(nuc,n) = FLOWQ(n-1) * WATC(nuc,n-1)
A12(nuc,n) = K1(nuc,n) + 1/DETIME(n)
A13(nuc,n) = K2(nuc,n)
A21(nuc,n) = 0
A22(nuc,n) = K1(nuc,n)
A23(nuc,n) = K2(nuc,n) + K3(nuc,n)

(equations on page 10-28)

Unit check:

A11 [m^3 a^{-1}] * [Bq m^{-3}] = [Bq a^{-1}]
A12 [a^{-1}] + 1 / [a] = [a^{-1}]
A13 [a^{-1}] = [a^{-1}]
A22 ([a^{-1}] = [a^{-1}]
A23 [a^{-1}] + [a^{-1}] = [a^{-1}]

KS(nuc,n) - KS PARAMETER USED IN WATEX [Bq]. Intermediate parameters used in the calculation of WATRW and WATRS in the WATEX module.

KW(nuc,n) - KW PARAMETER USED IN WATEX [Bq]. Intermediate parameters used in the calculation of WATRW and WATRS in the WATEX module.

Figure 3.3.8.2
Calculate KS PARAMETER
USED IN WATEX
(KS(nuc,n))
and
Figure 3.3.8.3
Calculate KW PARAMETER
USED IN WATEX
(KW(nuc,n))

$$\begin{tikzcd}
\text{LAKVOL(n)} \arrow[r, dashed] & \begin{matrix}\text{KS(nuc,n)}\\ \text{KW(nuc,n)}\end{matrix} & \begin{matrix}\text{A11(nuc,n),A21(nuc,n)}\\ \text{A12(nuc,n),A22(nuc,n)}\\ \text{A13(nuc,n),A23(nuc,n)}\end{matrix} \arrow[l]
\end{tikzcd}$$

Short Name	Long Name	SI Unit	Source
A11(nuc,n)A21(nuc,n)	MATRIX PARAMETERS USED IN WATEX	$[Bq\ a^{-1}]$	3.3.8.1
A12(nuc,n)A22(nuc,n) A13(nuc,n)A23(nuc,n)	MATRIX PARAMETERS USED IN WATEX	$[a^{-1}]$	3.3.8.1
KS(nuc,n)	KS PARAMETER USED IN WATEX	[Bq]	3.3.8.2
KW(nuc,n)	KW PARAMETER USED IN WATEX	[Bq]	3.3.8.3
LAKVOL(n)	VOLUME OF LAKE n	$[m^3]$	3.2.2

If LAKVOL(n) > 0

$$\text{KS(nuc,n)} = \frac{\text{A11(nuc,n)} * \text{A22(nuc,n)}}{\text{A12(nuc,n)} * \text{A23(nuc,n)} - \text{A13(nuc,n)} * \text{A22(nuc,n)}}$$

$$\text{KW(nuc,n)} = \frac{\text{A11(nuc,n)} * \text{A23(nuc,n)}}{\text{A12(nuc,n)} * \text{A23(nuc,n)} - \text{A22(nuc,n)} * \text{A13(nuc,n)}}$$

(pg. 10-28;
see Note 2)

Unit check:

KS $[Bq\ a^{-1}] * [a^{-1}] / ([a^{-1}] * [a^{-1}] - [a^{-1}] * [a^{-1}]) = [Bq]$

KW $[Bq\ a^{-1}] * [a^{-1}] / ([a^{-1}] * [a^{-1}] - [a^{-1}] * [a^{-1}]) = [Bq]$

Note 1: Dimensions do not agree with Table 10.5, which is probably incorrect.

Note 2: Inspection of the UTAP2 code shows that the numerators above for KS and KW are missing terms A12(nuc,n) * A21(nuc,n) and A13(nuc,n) * A21(nuc,n), respectively. Derivation of the equations shows that the UTAP2 code is correct and the SENES documentation is in error. The corrected equations are used in SYVAC3-UT2. (BWG, 87-04-09). Note that, since A21 is zero at all times, these "corrections" do not affect the results. (RJL, 87-05-03)

Figure 3.3.8.4
Calculate V1 PARAMETER
USED IN WATEX
(V1(nuc,n))
and
Figure 3.3.8.5
Calculate V2 PARAMETER
USED IN WATEX
(V2(nuc,n))

V1(nuc,n) - V1 PARAMETER USED IN WATEX [a^{-1}]. Intermediate parameter used in the calculation of WATRW and WATRS in the WATEX module.

V2(nuc,n) - V2 PARAMETER USED IN WATEX [a^{-1}]. Intermediate parameter used in the calculation of WATRW and WATRS in the WATEX module.

$$\begin{tikzcd}
\text{LAKVOL(n)} \arrow[r, dashed] & \begin{array}{l}\text{V1(nuc,n)}\\ \text{V2(nuc,n)}\end{array} & \begin{array}{l}\text{A11(nuc,n),A21(nuc,n)}\\ \text{A12(nuc,n),A22(nuc,n)}\\ \text{A13(nuc,n),A23(nuc,n)}\end{array} \arrow[l]
\end{tikzcd}$$

Short Name	Long Name	SI Unit	Source
A11(nuc,n)A21(nuc,n)	MATRIX PARAMETERS USED IN WATEX	[Bq a^{-1}]	3.3.8.1
A12(nuc,n)A22(nuc,n)	MATRIX PARAMETERS USED IN WATEX	[a^{-1}]	3.3.8.1
A13(nuc,n)A23(nuc,n)			
LAKVOL(n)	VOLUME OF LAKE n	[m^3]	3.2.2
V1(nuc,n)	V1 PARAMETER USED IN WATEX	[a^{-1}]	3.3.8.4
V2(nuc,n)	V2 PARAMETER USED IN WATEX	[a^{-1}]	3.3.8.5

If LAKVOL(n) > 0

$$V1(nuc,n) = \frac{- A12 - A23 + [(A12 + A23)^2 + 4 * (A13 * A22 - A12 * A23)]^{0.5}}{2}$$

$$V2(nuc,n) = \frac{- A12 - A23 - [(A12 + A23)^2 + 4 * (A13 * A22 - A12 * A23)]^{0.5}}{2}$$

(page 10-28)

Unit check: V1 and V2

$$\frac{[a^{-1}] - [a^{-1}] - [([a^{-1}] + [a^{-1}])^2 + 4\ ([a^{-1}] * [a^{-1}] - [a^{-1}] * [a^{-1}])]^{0.5}}{[-]}$$

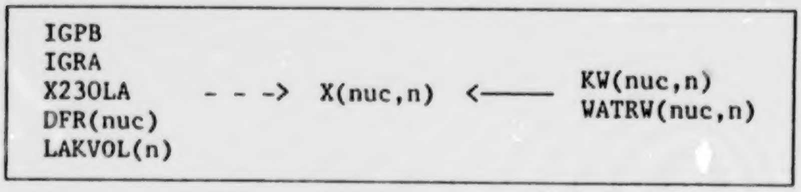
$$= [a^{-1}]$$

Note 1: The "-" sign in the equation in SENES Vol. 3 is for the first term only (SENES letter 1987-02-03).

Note 2: The "2" in the denominator and the "4" in the numerator are assumed to be dimensionless. The dimensions of V1 and V2 do not agree with Table 10.5, which is probably incorrect.

Figure 3.3.8.6
Calculate X PARAMETER
USED IN WATEX
(X(nuc,n))

X(nuc,n) - X PARAMETER USED IN WATEX [Bq]. Intermediate parameter used in the calculation of WATRW and WATRS in WATEX module.



Short Name	Long Name	SI Unit	Source
DFR(nuc)	RADIONUCLIDE DECAY FACTOR	[-]	3.3.7
IGPB	INGROWTH FACTOR FOR PB-210	[-]	1.5.1.1
IGRA	INGROWTH FACTOR FOR RA-226	[-]	1.4.1.1
KW(nuc,n)	KW PARAMETER USED IN WATEX	[Bq]	3.3.8.3
LAKVOL(n)	VOLUME OF LAKE n	[m^3]	3.2.2
WATRW(nuc,n)	QUANTITY OF RADIONUCLIDE IN LAKE WATER COL.	[Bq]	3.3.8.10
X(nuc,n)	X PARAMETER USED IN WATEX	[Bq]	3.3.8.6
X230LA	ACTIV. FRACT. TH-230 IN SOLU. TH	[-]	1.3.1.7B

(a) If LAKVOL(n) > 0

(i) if nuc = U, Th

$X(nuc,n)$ (at TIME=t) $= WATRW(nuc,n)_{t-\Delta t} - KW(nuc,n)$

(eqn. at bottom pg. 10-28)

(ii) if nuc = Ra

$X(Ra,n)$ (at TIME=t) $= WATRW(Ra,n)_{t-\Delta t} * DFR(Ra) + X230LA * WATRW(Th,n)_{t-\Delta t} * IGRA - KW(nuc,n)$

(see Notes 1,2)

(iii) if nuc = Pb

$X(Pb,n)$ (at TIME=t) $= WATRW(Pb,n)_{t-\Delta t} * DFR(Pb) + WATRW(Ra,n)_{t-\Delta t} * IGPB - KW(nuc,n)$

(see Notes 1,2)

(b) If LAKVOL(n) = 0, X(nuc,n) is not defined

Unit check(ii): X(Ra,n) [Bq] * [-] + [-] * [Bq] * [-] - [Bq] = [Bq]
and similarly for the other X terms

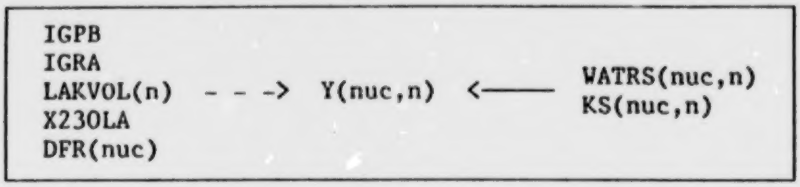
Note 1: The equations combine modified versions of those on page 10-30 (SENES letter (1986-12-02)) with the equation for $X_{i,t}$ on page 10-29.

Note 2: IGRA, IGPB, DFR(nuc) have been used to modify (simplify) the equations.

Note 3: Dimensions do not agree with Table 10.5 which is probably incorrect.

Y(nuc,n) - PARAMETER USED IN WATEX [Bq].
Intermediate parameter used in the calculation of WATRW and WATRS in the WATEX module.

Figure 3.3.8.7
Calculate Y PARAMETER USED IN WATEX (Y(nuc,n))



Short Name	Long Name	SI Unit	Source
DFR(nuc)	RADIONUCLIDE DECAY FACTOR	[-]	3.3.7
IGPB	INGROWTH FACTOR FOR PB-210	[-]	1.5.1.1
IGRA	INGROWTH FACTOR FOR RA-226	[-]	1.4.1.1
KS(nuc,n)	KS PARAMETER USED IN WATEX	[Bq]	3.3.8.2
LAKVOL(n)	VOLUME OF LAKE n	[m^3]	3.2.2
WATRS(nuc,n)	QUANTITY OF RADIONUCLIDE IN LAKE SEDIMENT EXCH. ZONE	[Bq]	3.3.8.11
X230LA	ACTIV. FRACT. TH-230 IN SOLU. TH	[-]	1.3.1.7B
Y(nuc,n)	Y PARAMETER USED IN WATEX	[Bq]	3.3.8.7

(a) If LAKVOL(n) > 0

(i) if nuc = U, Th

$$Y(nuc,n)\ (\text{at TIME}=t) = WATRS(nuc,n)_{t-\Delta t} - KS(nuc,n)$$

(eqn. at bottom page 10-28)

(ii) if nuc = Ra

$$Y(Ra,n)\ (\text{at TIME}=t) = WATRS(Ra,n)_{t-\Delta t} * DFR(Ra) + X230LA * WATRS(Th,n)_{t-\Delta t} * IGRA - KS(nuc,n)$$

(see Notes 1,2)

(iii) if nuc = Pb

$$Y(Pb,n)\ (\text{at TIME}=t) = WATRS(Pb,n)_{t-\Delta t} * DFR(Pb) + WATRS(Ra,n)_{t-\Delta t} * IGPB - KS(nuc,n)$$

(see Notes 1,2)

(b) If LAKVOL(n) = 0, Y(nuc,n) is not defined

Unit check (ii):
Y(Ra,n): [Bq] * [-] + [-] * [Bq] * [-] - [Bq] = [Bq]
and similarly for other Y terms

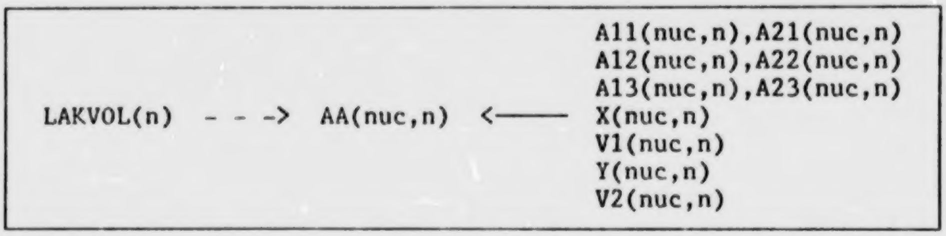
Note 1: The equations combine corrected versions of those on page 10-30 (SENES letter 1986-12-02) with the equation for $Y_{i,t}$ on page 10-29.

Note 2: IGRA, IGPB and DFR(nuc) have been used to modify (simplify) the equations.

Note 3: Dimensions do not agree with Table 10.5 which is probably incorrect.

AA(nuc,n) - AA PARAMETER USED IN WATEX [Bq]. Intermediate parameter used in the calculation of WATRW and WATRS in the WATEX module.

Figure 3.3.8.8
Calculate AA PARAMETER
USED IN WATEX
(AA(nuc,n))



Short Name	Long Name	SI Unit	Source
A11(nuc,n)A21(nuc,n)	MATRIX PARAMETERS USED IN WATEX	[Bq a^{-1}]	3.3.8.1
A12(nuc,n)A22(nuc,n) A13(nuc,n)A23(nuc,n)	MATRIX PARAMETERS USED IN WATEX	[a^{-1}]	3.3.8.1
AA(nuc,n)	AA PARAMETER USED IN WATEX	[Bq]	3.3.8.8
LAKVOL(n)	VOLUME OF LAKE n	[m^3]	3.2.2
V1(nuc,n)	V1 PARAMETER USED IN WATEX	[a^{-1}]	3.3.8.4
V2(nuc,n)	V2 PARAMETER USED IN WATEX	[a^{-1}]	3.3.8.5
X(nuc,n)	X PARAMETER USED IN WATEX	[Bq]	3.3.8.6
Y(nuc,n)	Y PARAMETER USED IN WATEX	[Bq]	3.3.8.7

If LAKVOL(n) > 0

$$AA(nuc,n) = \left[\frac{A13(nuc,n) + A23(nuc,n) + V1(nuc,n)}{A12(nuc,n) + A22(nuc,n) - (A13(nuc,n) + A23(nuc,n))}\right] *$$

$$\left\{\frac{[A12(nuc,n)+A22(nuc,n)+V2(nuc,n)]*X(nuc,n)-[A13(nuc,n)+A23(nuc,n)+V2(nuc,n)]*Y(nuc,n)}{[(A12(nuc,n)+A23(nuc,n))^2+4*(A13(nuc,n)*A22(nuc,n)-A12(nuc,n)*A23(nuc,n))]^{0.5}}\right\}$$

(eqn. top page 10-29)

Unit check:

$$\left\{\frac{([a^{-1}]+[a^{-1}]+[a^{-1}])}{[a^{-1}]+[a^{-1}]-([a^{-1}]+[a^{-1}])}\right\}*\left\{\frac{\{[a^{-1}]+[a^{-1}]+[a^{-1}]\}*[Bq]-\{[a^{-1}]+[a^{-1}]+[a^{-1}]\}*[Bq]}{[([a^{-1}]+[a^{-1}])^2+[-]*([a^{-1}]*[a^{-1}]-[a^{-1}]*[a^{-1}])]^{0.5}}\right\}$$

= [Bq]

Note: "4" has been assumed dimensionless. Dimensions do not agree with Table 10.5, which is probably incorrect.

BB(nuc,n) - BB PARAMETER USED IN WATEX [Bq]. Intermediate parameter used in the calculation of WATRW and WATRS in the WATEX module.

Figure 3.3.8.9
Calculate BB PARAMETER
USED IN WATEX
(BB(nuc,n))

```
                                      A11(nuc,n),A21(nuc,n)
                                      A12(nuc,n),A22(nuc,n)
LAKVOL(n)  - - ->  BB(nuc,n)  <———    A13(nuc,n),A23(nuc,n)
                                      AA(nuc,n)
                                      V1(nuc,n)
```

Short Name	Long Name	SI Unit	Source
A11(nuc,n)A21(nuc,n)	MATRIX PARAMETERS USED IN WATEX	[Bq a^{-1}]	3.3.8.1
A12(nuc,n)A22(nuc,n) A13(nuc,n)A23(nuc,n)	MATRIX PARAMETERS USED IN WATEX	[a^{-1}]	3.3.8.1
AA(nuc,n)	AA PARAMETER USED IN WATEX	[Bq]	3.3.8.8
BB(nuc,n)	BB PARAMETER USED IN WATEX	[Bq]	3.3.8.9
LAKVOL(n)	VOLUME OF LAKE n	[m^3]	3.2.2
V1(nuc,n)	V1 PARAMETER USED IN WATEX	[Bq]	3.3.8.4

If LAKVOL(n) > 0

$$BB(nuc,n) = \left(\frac{A12(nuc,n) + A22(nuc,n) + V1(nuc,n)}{A13(nuc,n) + A23(nuc,n) + V1(nuc,n)}\right) * AA(nuc,n)$$

Unit check:

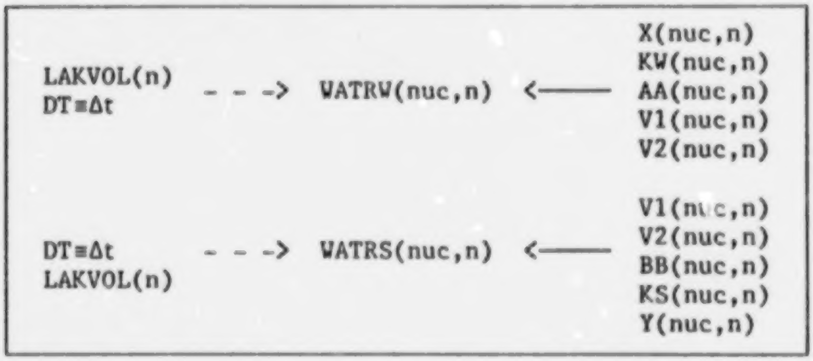
$$\left(\frac{[a^{-1}] + [a^{-1}] + [a^{-1}]}{[a^{-1}] + [a^{-1}] + [a^{-1}]}\right) * [Bq] = [Bq]$$

Note: Unit check does not agree with Table 10.5. Table 10.5 is probably incorrect.

WATRW(nuc,n) - QUANTITY OF RADIONUCLIDE IN LAKE WATER COLUMN [Bq]. Radionuclide activity in the water column of lake n (nuc = nat-U, tot-Th, Ra-226, Pb-210).

WATRS(nuc,n) - QUANTITY OF RADIONUCLIDE IN LAKE SEDIMENT EXCH. ZONE [Bq]. Radionuclide activity in the lake sediment exchange zone of lake n (nuc = nat-U, tot-Th, Ra-226, Pb-210).

Figure 3.3.8.10
Calculate QUANTITY OF RADIONUCLIDES IN LAKE WATER COL.
(WATRW(nuc,n))
and
Figure 3.3.8.11
Calculate QUANTITY OF RADIONUCLIDES IN LAKE SEDIMENT EXCH. ZONE
(WATRS(nuc,n))
(Page 1 of 2)



Short Name	Long Name	SI Unit	Source
AA(nuc,n)	AA PARAMETER USED IN WATEX	[Bq]	3.3.8.8
BB(nuc,n)	BB PARAMETER USED IN WATEX	[Bq]	3.3.8.9
DT≡Δt	TIME STEP-SIZE	[a]	Sampled
KS(nuc,n)	KS PARAMETER USED IN WATEX	[Bq]	3.3.8.2
KW(nuc,n)	KW PARAMETER USED IN WATEX	[Bq]	3.3.8.3
LAKVOL(n)	VOLUME OF LAKE n	[m^3]	3.2.2
V1(nuc,n)	V1 PARAMETER USED IN WATEX	[Bq]	3.3.8.4
V2(nuc,n)	V2 PARAMETER USED IN WATEX	[Bq]	3.3.8.5
WATRS(nuc,n)	QUANTITY OF RADIONUCLIDE IN LAKE SEDIMENT EXCH. ZONE	[Bq]	3.3.8.11
WATRW(nuc,n)	QUANTITY OF RADIONUCLIDE IN LAKE WATER COL.	[Bq]	3.3.8.10
X(nuc,n)	X PARAMETER USED IN WATEX	[Bq]	3.3.8.6
Y(nuc,n)	Y PARAMETER USED IN WATEX	[Bq]	3.3.8.7

If LAKVOL(n) > 0

WATRW(nuc,n) = KW(nuc,n) + AA(nuc,n) * EXP(V1(nuc,n) * DT)
+ (X(nuc,n) - AA(nuc,n)) * EXP(V2(nuc,n) * DT)

(eqn. 10.32; see Note 3)

WATRS(nuc,n) = KS(nuc,n) + BB(nuc,n) * EXP(V1(nuc,n) * DT)
+ (Y(nuc,n) - BB(nuc,n)) * EXP(V2(nuc,n) * DT)

(eqn. 10.33)

Unit check:

WATRW: $[Bq] + [Bq] * EXP([a^{-1}] * [a]) + ([Bq] - [Bq]) * EXP([a^{-1}] * [a]) = [Bq]$

WATRS: $[Bq] + [Bq] * EXP([a^{-1}] * [a]) + ([Bq] - [Bq]) * EXP([a^{-1}] * [a]) = [Bq]$

Figure 3.3.8.10
Calculate QUANTITY OF
RADIONUCLIDES IN LAKE
WATER COL.
(WATRW(nuc,n))
and
Figure 3.3.8.11
Calculate QUANTITY OF
RADIONUCLIDES IN LAKE
SEDIMENT EXCH. ZONE
(WATRS(nuc,n))
(Page 2 of 2)

Note 1: WATRW(nuc,n) = WATRS(nuc,n) = 0 at t=0 is assumed.

Note 2: These equations are a pair of coupled finite difference equations involving all equations shown in Figures 3.3.8.6, 3.3.8.7, 3.3.8.8, 3.3.8.9, 3.3.8.10 and 3.3.8.11 (see Figure 3.3.8).

Note 3: Inspection of the UTAP2 code shows that the exponential factors in the equations for WATRW and WATRS are calculated as follows:

```
if (V1 * DT) < -50 then exp. factor = 0
otherwise exp. factor = EXP (V1(nuc,n) * DT)
```

and similarly for V2. These modifications have been installed in SYVAC3-UT2. (BWG, 87-04-09)

Figure 3.3.9
Calculate CONC. OF RADIONUCLIDE IN WATER AT NODE n
(n-TC(nuc,n))

WATC(nuc,n) - CONCENTRATION OF RADIONUCLIDE IN WATER AT WATERSHED NODE N [Bq m^{-3}]. Concentration of radionuclide (nuc = nat-U, tot-Th, Ra-226, Pb-210) in the aqueous phase at node n of the watershed.

$$\begin{tikzcd} & & \text{WATC(nuc,n-1)} \\ \text{LAKVOL(n)} \arrow[r, dashed] & \text{WATC(nuc,n)} & \text{WATRW(nuc,n)} \arrow[l] \\ & & \text{FLOWQ(n)} \end{tikzcd}$$

Short Name	Long Name	SI Unit	Source
FLOWQ(n)	FLOW AT NODE n	[m^3 a^{-1}]	3.2.3
LAKVOL(n)	VOLUME OF LAKE n	[m^3]	3.2.2
WATC(nuc,n)	CONCENTRATION OF RADIONUCLIDE IN WATER AT WATERSHED NODE n	[Bq m^{-3}]	3.3.9
WATC(nuc,n-1)	CONCENTRATION OF RADIONUCLIDE IN WATER AT WATERSHED NODE (n-1) (n>1)	[Bq m^{-3}]	3.3.9
WATRW(nuc,n)	QUANTITY OF RADIONUCLIDE IN LAKE WATER COL.	[Bq]	3.3.8.10

For $n > 1$

If $\text{LAKVOL(n)} > 0$

$$\text{WATC(nuc,n)} = \frac{\text{WATRW(nuc,n)}}{\text{LAKVOL(n)}} \qquad \text{(eqn. 10.31)}$$

If $\text{LAKVOL(n)} = 0$

$$\text{WATC(nuc,n)} = \frac{\text{FLOWQ(n-1)} * \text{WATC(nuc,n-1)}}{\text{FLOWQ(n)}} \qquad \text{(eqn. 10.9, modified)}$$

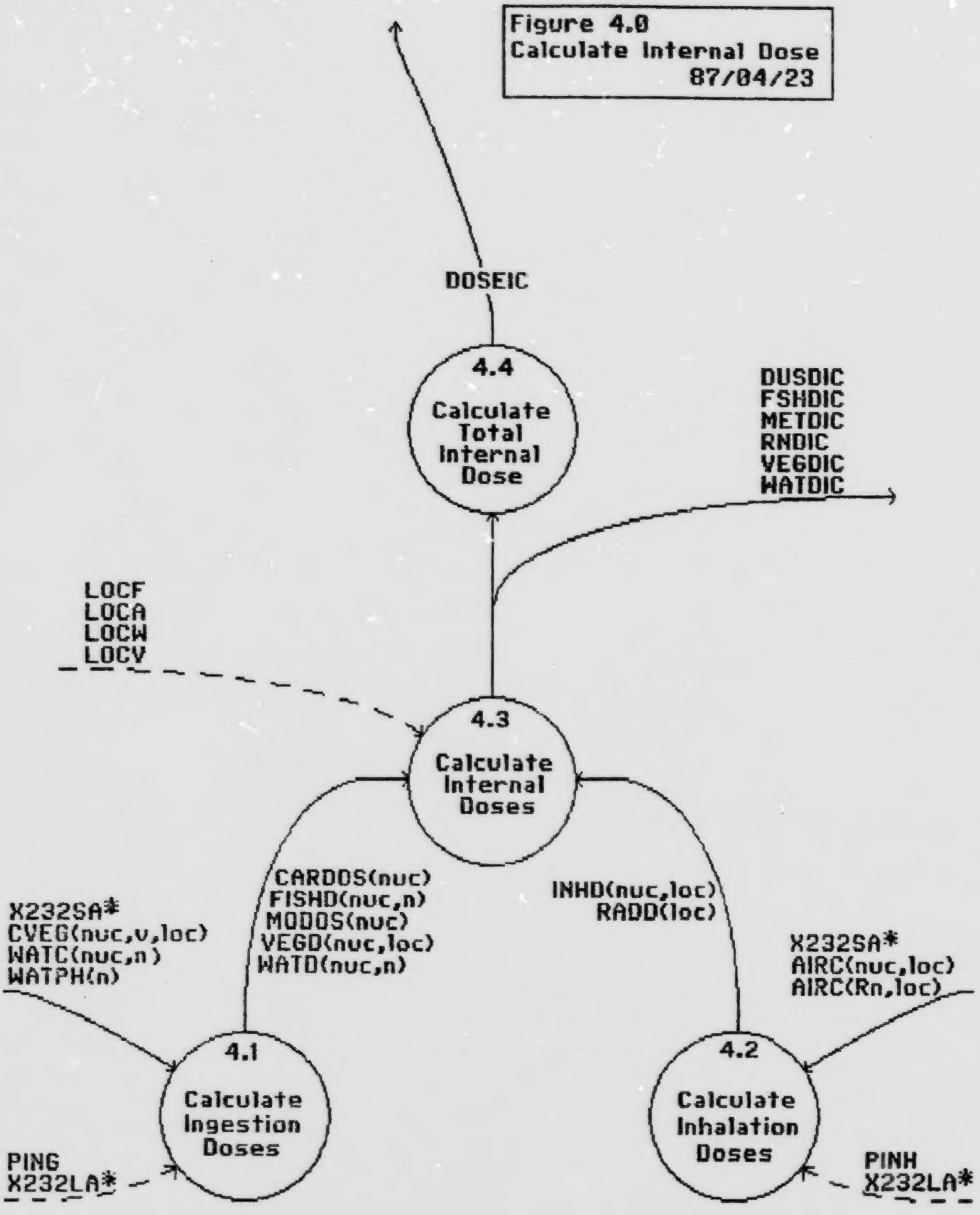
Unit check:

$$[\text{Bq}] \,/\, [\text{m}^3] = [\text{Bq m}^{-3}]$$

$$[\text{m}^3 \text{ a}^{-1}] * [\text{Bq m}^{-3}] \,/\, [\text{m}^3 \text{ a}^{-1}] = [\text{Bq m}^{-3}]$$

Note: Equation (10.9) has been modified so the source concentrations are not added at each step (see SENES letter 1986-10-15 for the resolution of a similar difficulty with equations (10.2) and (10.3)).

Figure 4.0
Calculate Internal Dose
87/04/23

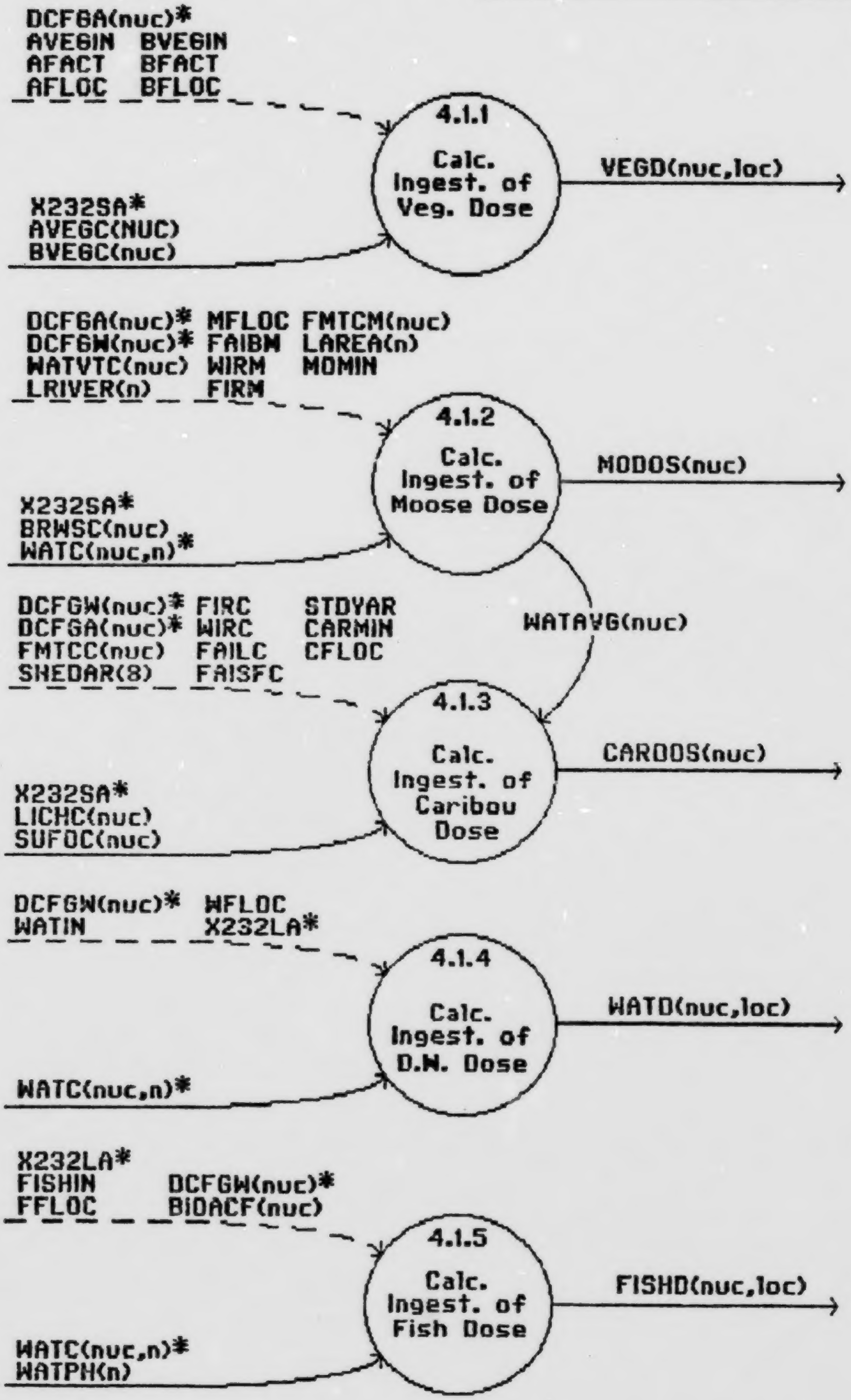

DOSEIC
4.4
Calculate Total Internal Dose
DUSDIC
FSHDIC
METDIC
RNDIC
VEGDIC
WATDIC
LOCF
LOCA
LOCW
LOCV
4.3
Calculate Internal Doses
CARDOS(nuc)
FISHD(nuc,n)
MODOS(nuc)
VEGD(nuc,loc)
WATD(nuc,n)
INHD(nuc,loc)
RADD(loc)
X232SA*
CVEG(nuc,v,loc)
WATC(nuc,n)
WATPH(n)
X232SA*
AIRC(nuc,loc)
AIRC(Rn,loc)
4.1
Calculate Ingestion Doses
4.2
Calculate Inhalation Doses
PING
X232LA*
PINH
X232LA*

Note 1. PING and PINH are two sets of sampled parameters; refer to the data dictionary for their contents.

2. nuc = nat. U, tot. Th, Pb-210 and Ra-226 in this and the lower level figures.

3. This figure and its lower level figures apply to the calculation of internal dose to a critical receptor (DOSEIC, VEGDIC, etc.). An identical set of figures would apply to internal dose to an average receptor (DOSEIA, VEGDIA, etc.), execpt for the use of different values (and/or distributions) for some parameters. These parameters are identified in the DDDs below.

Figure 4.1
Calculate Ingestion Doses
87/04/23


DCFGA(nuc)*
AVEGIN BVEGIN
AFACT BFACT
AFLOC BFLOC
4.1.1
Calc. Ingest. of Veg. Dose
VEGD(nuc,loc)
X232SA*
AVEGC(NUC)
BVEGC(nuc)
DCFGA(nuc)* MFLOC FMTCM(nuc)
DCFGW(nuc)* FAIBM LAREA(n)
WATVTC(nuc) WIRM MOMIN
LRIVER(n) FIRM
4.1.2
Calc. Ingest. of Moose Dose
MODOS(nuc)
X232SA*
BRWSC(nuc)
WATC(nuc,n)*
WATAVG(nuc)
DCFGW(nuc)* FIRC STDYAR
DCFGA(nuc)* WIRC CARMIN
FMTCC(nuc) FAILC CFLOC
SHEDAR(8) FAISFC
4.1.3
Calc. Ingest. of Caribou Dose
CARDOS(nuc)
X232SA*
LICHC(nuc)
SUFOC(nuc)
DCFGW(nuc)* WFLOC
WATIN X232LA*
4.1.4
Calc. Ingest. of D.W. Dose
WATD(nuc,loc)
WATC(nuc,n)*
X232LA*
FISHIN DCFGW(nuc)*
FFLOC BIOACF(nuc)
4.1.5
Calc. Ingest. of Fish Dose
FISHD(nuc,loc)
WATC(nuc,n)*
WATPH(n)

Note: DCFGW(Th) and DCFGA(Th) are calculated parameters.

Figure 4.1.1
Calculate INGEST. OF VEG. DOSE (VEGD(nuc,loc))

VEGD(nuc,loc) - INGEST. OF VEG. DOSE [$\mu Sv\ a^{-1}$]. The average annual whole body dose due to ingestion of above- and below-ground vegetables for radionuclide nuc (nuc = nat-U, tot-Th, Ra-226 and Pb-210).

DCFGA(nuc)
AVEGIN
BVEGIN
AFACT - - -> VEGD(nuc,loc) <—— DCFGA(tot-Th), AVEGC(nuc,loc), BVEGC(nuc,loc)
BFACT
AFLOC
BFLOC

DCFGA(tot-Th) <—— X232SA

Short Name	Long Name	SI Unit	Source
AFACT	FRAC. OF ACTIVITY IN VEG. TYPE A	[-]	Sampled
AFLOC	FRAC. OF VEG. TYPE A LOCALLY GROWN	[-]	Sampled
AVEGC(nuc,loc)	CONC. OF RADIONUCLIDE IN ABOVE-GROUND VEGETABLES	[$Bq\ g^{-1}$]	2.6
AVEGIN	AV. INTAKE OF VEG. TYPE A	[$g\ a^{-1}$]	Sampled
BFACT	FRAC. OF ACTIVITY IN VEG. TYPE B	[-]	Sampled
BFLOC	FRAC. OF VEG. TYPE B LOCALLY GROWN	[-]	Sampled
BVEGC(nuc,loc)	CONC. OF RADIONUCLIDE IN BELOW-GROUND VEGETABLES	[$Bq\ g^{-1}$]	2.6
BVEGIN	AV. INTAKE OF VEG. TYPE B	[$g\ a^{-1}$]	Sampled
DCFGA(nuc)	DCF FOR INGESTION OF NUC (AIR)	[$\mu Sv\ Bq^{-1}$]	Sampled
DCFGA(tot-Th)	DCF FOR INGESTION OF TH (AIR)	[$\mu Sv\ Bq^{-1}$]	(4.1.1)
VEGD(nuc,loc)	INGEST. OF VEG. DOSE	[$\mu Sv\ a^{-1}$]	4.1.1
X232SA	ACT. FRACT. TH-232 IN SURF. SOLID TH	[-]	1.3.2.5C

$$\text{DCFGA(tot-Th)} = 1.5\ 10^{-1} + \text{X232SA} * (6.9 \times 10^{-1}) \qquad \text{(Table 13.2)}$$

$$\text{VEGD(nuc,loc)} = \text{DCFGA(nuc)} * \{\text{AVEGIN} * \text{AVEGC(nuc,loc)} * \text{AFACT} * \text{AFLOC} + \text{BVEGIN} * \text{BVEGC(nuc,loc)} * \text{BFACT} * \text{BFLOC}\} \qquad \text{(eqn. 13.1)}$$

Unit check:

DCFGA(tot-Th): not possible; no units given in Table 13.2

$$\text{VEGD: } [\mu Sv\ Bq^{-1}] * \{[g(wet)\ a^{-1}] * [Bq\ g^{-1}(wet)] * [-] * [-]\} = [\mu Sv\ a^{-1}]$$

Note 1: For the average receptor, AVEGIN, BVEGIN, AFLOC and BFLOC are sampled from different distributions; see SENES Vol. 3, Tables 13.3 and 13.4.

Note 2: VEGD, AVEGC and BVEGC are location-dependant.

Note 3: For nuc = total thorium, DCFGA(nuc) is not a sampled parameter, but calculated using the equation shown. For nuc = natural uranium, Ra-226 and Pb-210, DCFGA(nuc) is sampled.

Note 4: It is assumed that R_v (page 13-6) and R_{vr} (Tables 13.3 and 13.4) are identical (and equivalent to AFACT and BFACT).

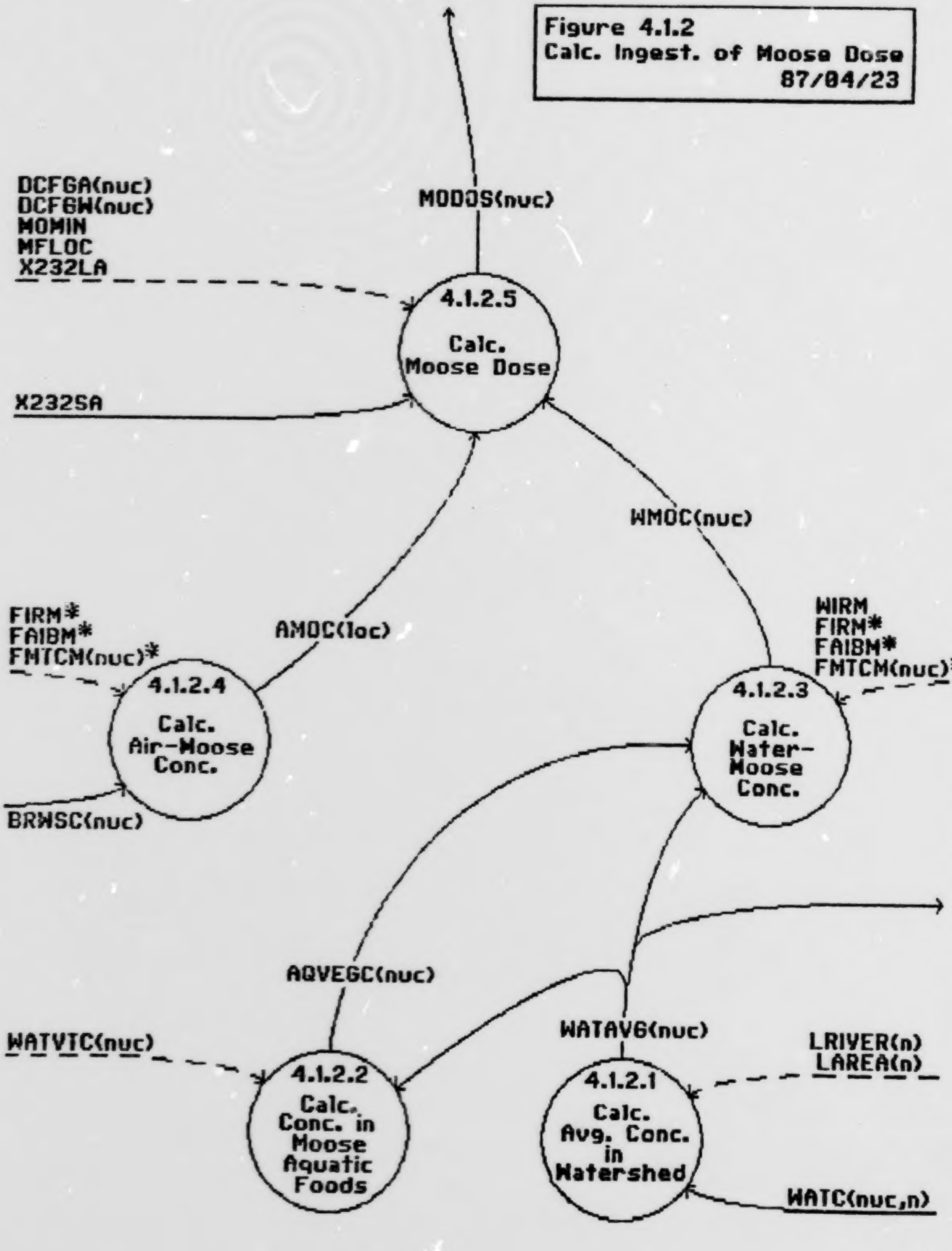


Figure 4.1.2
Calc. Ingest. of Moose Dose
87/04/23

MODOS(nuc)
DCFGA(nuc)
DCFGW(nuc)
MOMIN
MFLOC
X232LA
4.1.2.5
Calc.
Moose Dose
X232SA
WMOC(nuc)
AMOC(loc)
FIRM*
FAIBM*
FMTCM(nuc)*
4.1.2.4
Calc.
Air-Moose
Conc.
BRWSC(nuc)
WIRM
FIRM*
FAIBM*
FMTCM(nuc)*
4.1.2.3
Calc.
Water-
Moose
Conc.
AQVEGC(nuc)
WATAVG(nuc)
WATVTC(nuc)
4.1.2.2
Calc.
Conc. in
Moose
Aquatic
Foods
LRIVER(n)
LAREA(n)
4.1.2.1
Calc.
Avg. Conc.
in
Watershed
WATC(nuc,n)

Note: DCFGA(Th) and DCFGW(Th) are calculated parameters.

WATAVG(nuc) - AVG. CONC. IN WATERSHED [Bq m^{-3}]. The average concentration of radionuclide "nuc" (nuc= U-nat, Th-tot, Ra-226, Pb-210) along the edge of lakes and rivers in the watershed.

Figure 4.1.2.1
Calculate AVG. CONC.
IN WATERSHED
(WATAVG(nuc))

LRIVER(n)
LAREA(n) - - -> WATAVG(nuc) <—— WATC(nuc,n)

Short Name	Long Name	SI Unit	Source
LAREA(n)	AREA OF LAKE	[m^2]	Sampled
LRIVER(n)	LENGTH OF RIVER SEG.	[m]	Sampled
WATAVG(nuc)	AVG. CONC. IN WATERSHED	[Bq m^{-3}]	4.1.2.1
WATC(nuc,n)	CONCENTRATION OF RADIONUCLIDE IN WATER AT WATERSHED NODE N	[Bq m^{-3}]	3.3.6 & 3.3.9

$$\text{WATAVG(nuc)} = \frac{\sum\limits_{\substack{\text{nodes}\\ n}} \text{WATC(nuc,n)} * \left\{\text{LRIVER(n)} + (4\pi \times \text{LAREA(n)})^{1/2}\right\}}{\sum\limits_{\substack{\text{nodes}\\ n}} \left\{\text{LRIVER(n)} + (4\pi \times \text{LAREA(n)})^{1/2}\right\}}$$

(eqn. 11.4)

Unit check:

$$\Sigma\ [\text{Bq m}^{-3}] * \{[\text{m}] + [-] * ([-] * [\text{m}^2])^{1/2}\}\ /$$
$$\Sigma\ \{[\text{m}] + ([-] * [-] * [\text{m}^2])^{1/2}\}$$
$$= [\text{Bq m}^{-3}]$$

Note 1: Assumes $[\bar{R}_i]_t = [R_i]_t$ in eqn. (11.4) and Table 11.5.

Note 2: The factor 4π is assumed to be dimensionless and is a circumference factor (see SENES, Vol. 3, pg. 11-10).

Note 3: Assumes $S_n \neq$ LAREA(n) in Table 11.5; rather it is LRIVER - see columns 3 and 5 in Table 10.1.

Figure 4.1.2.2
Calculate CONC. IN
MOOSE AQUATIC FOODS
(AQVEGC(nuc))

AQVEGC(nuc) - CONC. IN MOOSE AQUATIC FOODS ($Bq \cdot g^{-1}$ (wet)]. The concentration of radionuclide "nuc" (nuc = U-nat, Th=tot, Ra-226, Pb-210) in aquatic vegetation consumed by moose.

WATVTC(nuc) - - -> AQVEGC(nuc) <—— WATAVG(nuc)

Short Name	Long Name	SI Unit	Source
AQVEGC(nuc)	CONC. IN MOOSE AQUATIC FOODS	$[Bq\ g^{-1}]$	4.1.2.2
WATAVG(nuc)	AVG. CONC. IN WATERSHED	$[Bq\ m^{-3}]$	4.1.2.1
WATVTC(nuc)	WATER-AQ. VEG. XFR COEFF.	$[m^3\ g^{-1}]$	Sampled

AQVEGC(nuc) = WATVTC(nuc) * WATAVG(nuc) (eqn. 11.3)

Unit check:

$$[Bq\ g^{-1}\ (wet) \cdot Bq^{-1}\ m^3] * [Bq\ m^{-3}]$$
$$= [Bq\ g^{-1}\ (wet)]$$

Note: Assumes $[R_i]_t = [\bar{R}_i]_t$ in eqn. 11.3 and Table 11.5.

Figure 4.1.2.3
Calculate WATER-MOOSE
CONC.
(WMOC(nuc))

WMOC(nuc) - WATER-MOOSE CONC. [Bq g^{-1} (wet)]. Concentration of the radionuclide "nuc" in moose flesh due to the water pathway (nuc = U-nat, Th-tot, Ra-226, Pb-210).

```
FMTCM(nuc)
FIRM          - - ->  WMOC(nuc)  <-----  WATAVG(nuc)
FAIAM                                    AQVEGC(nuc)
WIRM

FAIBM         - - ->  FAIAM
```

Short Name	Long Name	SI Unit	Source
AQVEGC(nuc)	CONC. IN MOOSE AQUATIC FOODS	[Bq g^{-1}]	4.1.2.2
FAIAM	MOOSE AQUATIC FRACTION	[-]	(4.1.2.3)
FAIBM	MOOSE BROWSE FRACTION	[-]	Sampled
FIRM	FEED RATE FOR MOOSE	[g d^{-1}]	Sampled
FMTCM(nuc)	MOOSE XFR COEFF.	[d g^{-1}]	Sampled
WATAVG(nuc)	AVG. CONC. IN WATERSHED	[Bq m^{-3}]	4.1.2.1
WIRM	MOOSE WATER INTAKE RATE	[m^3 d^{-1}]	Sampled
WMOC(nuc)	WATER-MOOSE CONC.	[Bq g^{-1}]	4.1.2.3

FAIAM = 1.0 - FAIBM (eqn. below eqn. 12.4)

WMOC(nuc) = FMTCM(nuc) * {FIRM * FAIAM * AQVEGC(nuc) + WIRM * WATAVG(nuc))} (eqn. 12.4)

Unit check:

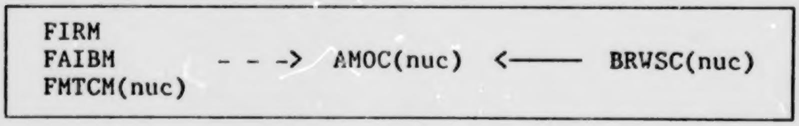
FAIAM: [-] - [-] = [-]

WMOC(nuc): [Bq g^{-1} (wet) · Bq^{-1} d] * {[g(wet) d^{-1}] * [-] * [Bq g^{-1} (wet)] + [m^3 d^{-1}] * [Bq m^{-3}]}
= [Bq g^{-1} (wet)]

Note: In the unit check, the units g(wet) may refer to flesh or vegetables; compare with SENES equation (12.4).

Figure 4.1.2.4
Calculate AIR-MOOSE
CONC.
(AMOC(nuc))

AMOC(nuc) - AIR-MOOSE CONC. [Bq g^{-1} (wet weight)]. Concentration of the radionuclide "nuc" in moose flesh due to the air pathway (nuc = U-nat, Th-tot, Ra-226, Pb-210).



Short Name	Long Name	SI Unit	Source
AMOC(nuc)	AIR-MOOSE CONC.	[Bq g^{-1}]	4.1.2.4
BRWSC(nuc)	CONC. OF RADIONUCLIDE IN BROWSE VEGETATION	[Bq g^{-1}]	2.6
FAIBM	MOOSE BROWSE FRAC.	[-]	Sampled
FIRM	FEED RATE FOR MOOSE	[g d^{-1}]	Sampled
FMTCM(nuc)	MOOSE XFR COEFF.	[d g^{-1}]	Sampled

$$\mathrm{AMOC(nuc)} = \mathrm{FMTCM(nuc)} * \mathrm{FIRM} * \mathrm{FAIBM} * \mathrm{BRWSC(nuc)} \qquad \text{(eqn. 12.3)}$$

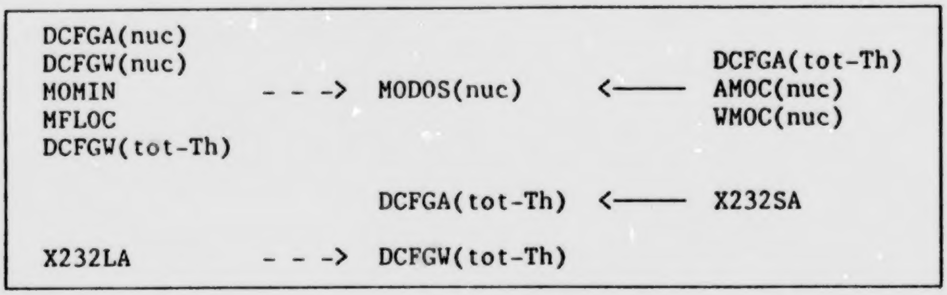
Unit check:

$$[\mathrm{Bq\ g^{-1}(wet)} \cdot \mathrm{Bq^{-1}\ d}] * [\mathrm{g(wet)\ d^{-1}}] * [-]$$
$$* [\mathrm{Bq\ g^{-1}(wet)}] = [\mathrm{Bq\ g^{-1}(wet)}]$$

Figure 4.1.2.5
Calculate MOOSE DOSE

(MODOS(nuc))

MODOS(nuc) - MOOSE DOSE [μSv a^{-1}].
Annual average whole body dose of radionuclide "nuc" (nuc = nat-U, tot-Th, Ra-226, Pb-210) from ingestion of moose meat for a specific location and receptor type.



Short Name	Long Name	SI Unit	Source
AMOC(nuc)	AIR-MOOSE CONC.	[Bq g^{-1}]	4.1.2.4
DCFGA(nuc)	DCF FROM INGEST. OF NUC (AIR)	[μSv Bq^{-1}]	Sampled
DCFGA(tot-Th)	DCF FROM INGEST. OF TH (AIR)	[μSv Bq^{-1}]	(4.1.2.5)
DCFGW(nuc)	DCF FROM INGEST. OF NUC. (WATER)	[μSv Bq^{-1}]	Sampled
DCFGW(tot-Th)	DCF FROM INGEST. OF TH (WATER)	[μSv Bq^{-1}]	(4.1.2.5)
MFLOC	FRAC. OF MOOSE LOCAL	[-]	Sampled
MODOS(nuc)	MOOSE DOSE	[μSv a^{-1}]	4.1.2.5
MOMIN	ANN. INTAKE OF MOOSE	[g a^{-1}]	Sampled
WMOC(nuc)	WATER-MOOSE CONC.	[Bq g^{-1}]	4.1.2.3
X232LA	ACTIV. FRACT. TH-232 IN SOLU. TH	[-]	1.3.1.7A
X232SA	ACT. FRACT. TH-232 IN SURF. SOLID TH	[-]	1.3.2.5C

$$\mathrm{DCFGA(tot\text{-}Th)} = 1.5 \times 10^{-1} + \mathrm{X232SA} * (6.9 \times 10^{-1}) \qquad \text{(Table 13.2)}$$

$$\mathrm{DCFGW(tot\text{-}Th)} = 1.5 \times 10^{-1} + \mathrm{X232LA} * (6.9 \times 10^{-1}) \qquad \text{(Table 13.2)}$$

$$\mathrm{MODOS(nuc)} = \mathrm{MOMIN} * \mathrm{MFLOC} * \begin{Bmatrix} \mathrm{DCFGA(nuc)} * \mathrm{AMOC(nuc)}\ + \\ \mathrm{DCFGW(nuc)} * \mathrm{WMOC(nuc)} \end{Bmatrix} \qquad \text{(eqn. 13.3)}$$

Unit check:

DCFGA(tot-Th) and DCFGW(tot-Th): not possible, no units given in Table 13.2

$$\mathrm{MODOS(nuc)}:\ [\mathrm{g(wet)\ a^{-1}}] * [-] * \begin{Bmatrix} [\mu\mathrm{Sv\ Bq^{-1}}] * [\mathrm{Bq\ g^{-1}(wet)}]\ + \\ [\mu\mathrm{Sv\ Bq^{-1}}] * [\mathrm{Bq\ g^{-1}(wet)}] \end{Bmatrix}$$

$$= [\mu\mathrm{Sv\ a^{-1}}]$$

Note 1: For the average receptor, MOMIN and MFLOC are sampled from different distributions; see SENES Vol. 3, Tables 13.3 and 13.4.

Note 2: MODOS(nuc) is apparently not location-specific, since WMOC(nuc) and AMOC(nuc) are "watershed area" averages. See text in SENES Vol. 3, p. 13-10 to 13-11.

Note 3: For nuc = total thorium, DCFGA(nuc) and DCFGW(nuc) are not sampled but calculated parameters, using the equations shown. They are sampled parameters for nuc = natural uranium, Ra-226 and Pb-210.

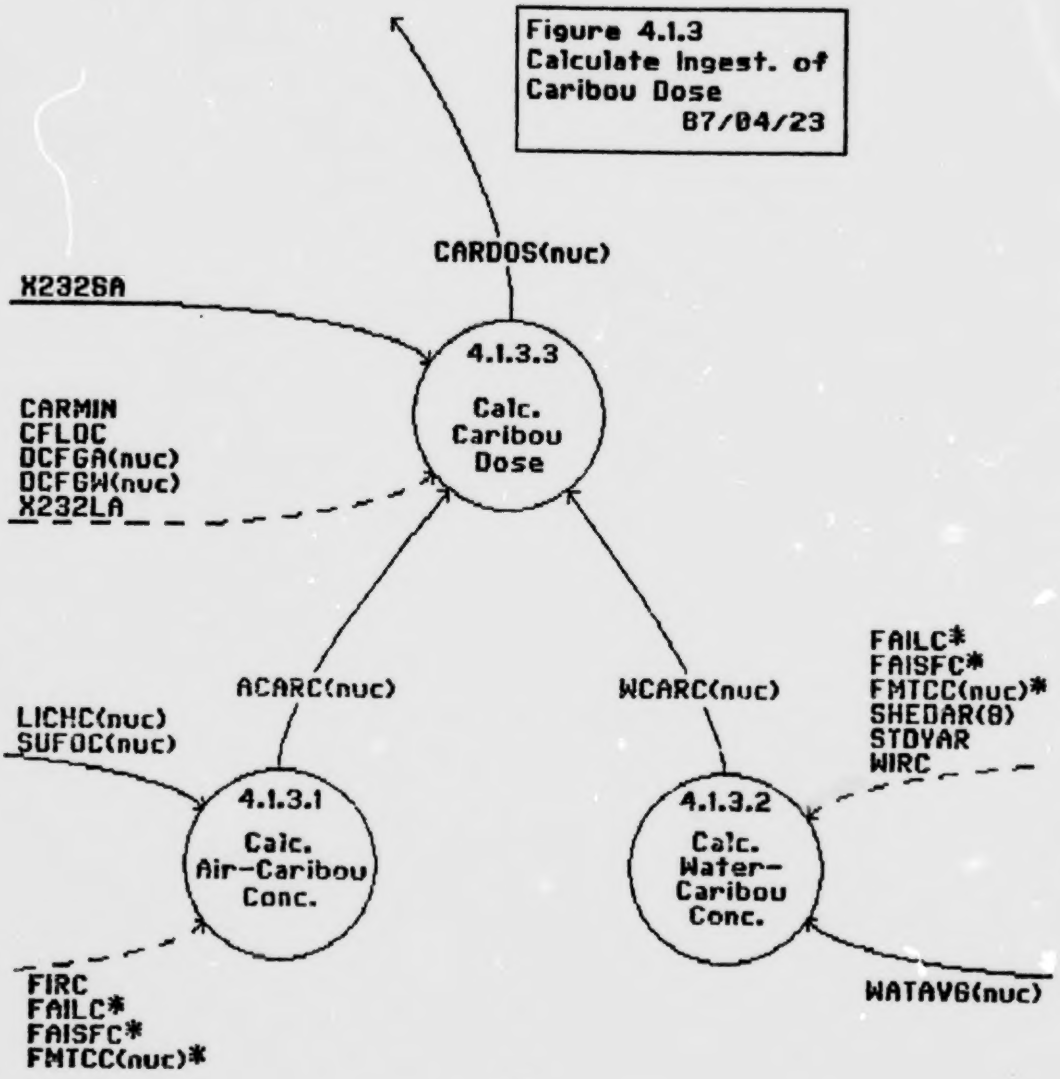


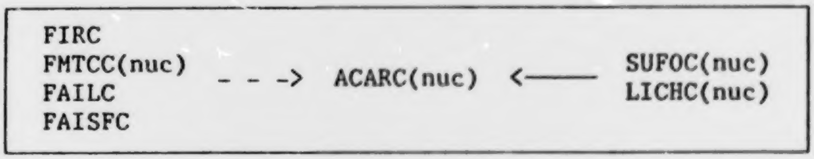
Figure 4.1.3
Calculate Ingest. of
Caribou Dose
87/04/23

CARDOS(nuc)
X232GA
4.1.3.3
Calc.
Caribou
Dose
CARMIN
CFLOC
DCFGA(nuc)
DCFGW(nuc)
X232LA
ACARC(nuc)
WCARC(nuc)
FAILC*
FAISFC*
FMTCC(nuc)*
SHEDAR(8)
STDVAR
WIRC
LICHC(nuc)
SUFOC(nuc)
4.1.3.1
Calc.
Air-Caribou
Conc.
4.1.3.2
Calc.
Water-
Caribou
Conc.
FIRC
FAILC*
FAISFC*
FMTCC(nuc)*
WATAVG(nuc)

Note: DCFGA(Th) and DCFGW(Th) are calculated parameters.

Figure 4.1.3.1
Calculate AIR-CARIBOU CONC.
(ACARC(nuc))

ACARC(nuc) - AIR-CARIBOU CONC. [Bq g^{-1}(wet)]. Concentration of the radionuclide "nuc" in caribou flesh due to the air pathway (nuc = U-nat, Th-tot, Ra-226, Pb-210).



Short Name	Long Name	SI Unit	Source
ACARC(nuc)	AIR-CARIBOU CONC.	[Bq g^{-1}]	4.1.3.1
FAILC	FRAC. OF INTAKE-LICHEN	[-]	Sampled
FAISFC	FRAC. OF INTAKE-FORAGE	[-]	Sampled
FIRC	FEED RATE FOR CARIBOU	[g d^{-1}]	Sampled
FMTCC(nuc)	CARIBOU XFR COEFF.	[d g^{-1}]	Sampled
LICHC(nuc)	CONC. OF RADIONUCLIDES IN LICHENS	[Bq g^{-1}]	2.6
SUFOC(nuc)	CONC. OF RADIONUCLIDE IN SUMMER FORAGE VEGETATION	[Bq g^{-1}]	2.6

$$\mathrm{ACARC(nuc)} = \mathrm{FIRC} * \mathrm{FMTCC(nuc)} * \{\mathrm{FAILC} * \mathrm{LICHC(nuc)} + \mathrm{FAISFC} * \mathrm{SUFOC(nuc)}\}$$

Unit check:

$[\mathrm{g(wet)}\ \mathrm{d}^{-1}] * [\mathrm{Bq}\ \mathrm{g}^{-1}\mathrm{(wet)} \cdot \mathrm{Bq}^{-1}\ \mathrm{d}] *$
$\{[-] * [\mathrm{Bq}\ \mathrm{g}^{-1}\mathrm{(wet)}] + [-] * [\mathrm{Bq}\ \mathrm{g}^{-1}\mathrm{(wet)}]\}$
$= [\mathrm{Bq}\ \mathrm{g}^{-1}\mathrm{(wet)}]$

Figure 4.1.3.2
Calculate WATER-CARIBOU CONC.
(WCARC(nuc))

WCARC(nuc) - WATER-CARIBOU CONC. [Bq g^{-1}(wet)]. Concentration of the radionuclide "nuc" in caribou flesh due to the water pathway (nuc = U-nat, Th-tot, Ra-226. Pb-210).

```
FT
WIRC
FMTCC(nuc)  - - ->  WCARC(nuc)  <———  WATAVG(nuc)
FAILC
FAISFC

SHEDAR(8)
STDYAR      - - ->  FT
```

Short Name	Long Name	SI Unit	Source
FAILC	FRAC. OF INTAKE-LICHEN	[-]	Sampled
FAISFC	FRAC. OF INTAKE-FORAGE	[-]	Sampled
FMTCC(nuc)	CARIBOU XFR COEFF.	[d g^{-1}]	Sampled
FT	WATERSHED ADJUSTMENT FACTOR	[-]	(4.1.3.2)
SHEDAR(8)	WATERSHED AREA	[m^2]	Sampled
STDYAR	STUDY AREA	[m^2]	Sampled
WATAVG(nuc)	AVG. CONC. IN WATERSHED	[Bq m^{-3}]	4.1.2.1
WCARC(nuc)	WATER-CARIBOU CONC.	[Bq g^{-1}]	4.1.3.2
WIRC	CARIBOU WATER INTAKE RATE	[m^3 d^{-1}]	Sampled

FT = SHEDAR(8) / STDYAR (see Note)

WCARC(nuc) = WIRC * FMTCC(nuc) * WATAVG(nuc) * FT * (FAILC + FAISFC) (eqn. 12.2)

Unit check:

FT: $[m^2] / [m^2] = [-]$

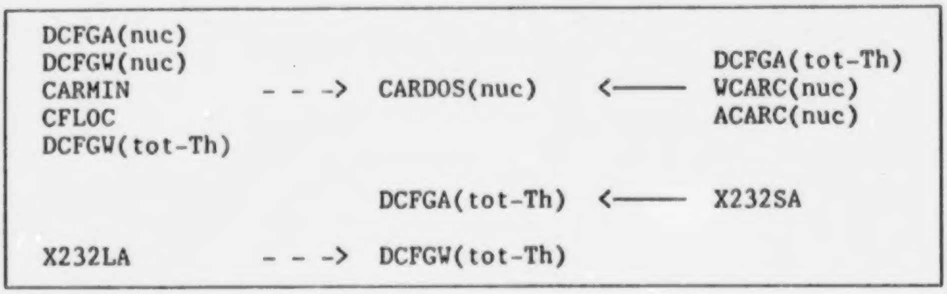
WCARC(nuc): $[m^3\ d^{-1}] * [\mathrm{Bq}\ g^{-1}(\mathrm{wet}) \cdot \mathrm{Bq}^{-1}\ d] * [\mathrm{Bq}\ m^{-3}] * [-]\ ([-] + [-])$
$= [\mathrm{Bq}\ g^{-1}(\mathrm{wet})]$

Note: The equation for FT was taken from the description on pages 12-3 and 12-6 of SENES Vol. 3. The description is not entirely clear, but appears to be reasonable. SENES does not define STDYAR as an input parameter, but they describe a "study area" on page 2-2 and in figures 2-2 and 10-1 as the area enclosed by a circle with a radius of 50 km. SHEDAR(8) is the (total) cumulative watershed area.

Figure 4.1.3.3
Calculate CARIBOU DOSE

(CARDOS(nuc))

CARDOS(nuc) - CARIBOU DOSE [$\mu Sv\ a^{-1}$]. Average annual whole body dose of radionuclide "nuc" (nuc = nat-U, tot-Th, Ra-226, Pb-210) from ingestion of caribou meat for a specific location and receptor type.



Short Name	Long Name	SI Unit	Source
ACARC(nuc)	AIR-CARIBOU CONC.	[$Bq\ g^{-1}$]	4.1.3.1
CARDOS(nuc)	CARIBOU DOSE	[$\mu Sv\ a^{-1}$]	4.1.3.3
CARMIN	ANN. INTAKE OF CARIBOU	[$g\ a^{-1}$]	Sampled
CFLOC	FRAC. OF CAR. LOCAL	[-]	Sampled
DCFGA(nuc)	DCF FROM INGEST. OF NUC (AIR)	[$\mu Sv\ Bq^{-1}$]	Sampled
DCFGA(tot-Th)	DCF FROM INGEST. OF TH (AIR)	[$\mu Sv\ Bq^{-1}$]	(4.1.3.3)
DCFGW(nuc)	DCF FROM INGEST. OF NUC (WATER)	[$\mu Sv\ Bq^{-1}$]	Sampled
DCFGW(tot-Th)	DCF FROM INGEST. OF TH (WATER)	[$\mu Sv\ Bq^{-1}$]	(4.1.3.3)
WCARC(nuc)	WATER-CARIBOU CONC.	[$Bq\ g^{-1}$]	4.1.3.2
X232LA	ACTIV. FRACT. TH-232 IN SOLU. TH	[-]	1.3.1.7A
X232SA	ACT. FRACT. TH-232 IN SURF. SOLID TH	[-]	1.3.2.5C

$$\text{DCFGA(tot-Th)} = 1.5 \times 10^{-1} + \text{X232SA} * (6.9 \times 10^{-1}) \qquad \text{(Table 13.2)}$$

$$\text{DCFGW(tot-Th)} = 1.5 \times 10^{-1} + \text{X232LA} * (6.9 \times 10^{-1}) \qquad \text{(Table 13.2)}$$

$$\text{CARDOS(nuc)} = \text{CARMIN} * \text{CFLOC} * \left\{ \begin{matrix} \text{DCFGA(nuc)} * \text{ACARC(nuc)} + \\ \text{DCFGW(nuc)} * \text{WCARC(nuc)} \end{matrix} \right\} \qquad \text{(eqn. 13.2)}$$

Unit check:

DCFGA(tot-Th) and DCFGW(tot-Th): not possible; no units given in Table 13.2.

$$\text{CARDOS(nuc)}: \quad [g(\text{wet})\ a^{-1}] * [-] * \left\{ \begin{matrix} [\mu Sv\ Bq^{-1}] * [Bq\ g^{-1}(\text{wet})] \\ + \\ [\mu Sv\ Bq^{-1}] * [Bq\ g^{-1}(\text{wet})] \end{matrix} \right\}$$

$$= [\mu Sv\ a^{-1}]$$

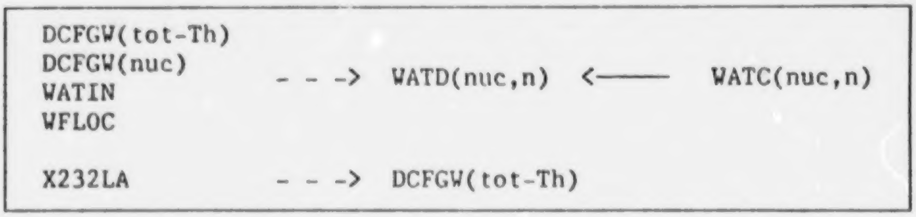
Note 1: For the average receptor, CARMIN and CFLOC are sampled from different distributions; see SENES Vol. 3, Tables 13.3 and 13.4.

Note 2: CARDOS(nuc) is not really location-specific, since ACARC(nuc) and WCARC(nuc) are "whole model area" averages. See text in SENES Vol. 3, p. 13-8 to 13-9.

Note 3: For nuc = total thorium only, DCFGA(nuc) and DCFGW(nuc) are calculated as shown. For nuc = U, Ra and Pb, these are sampled (input) parameters.

Figure 4.1.4
Calculate INGEST. OF D.W. DOSE (WATD(nuc,n))

WATD(nuc,n) - INGEST. OF D.W. DOSE [μSv a^{-1}]. Average annual whole body dose of radionuclide "nuc" (nuc = nat-U, tot-Th, Ra-226, Pb-210) from ingestion of water from the watershed for a specific location and receptor type.



Short Name	Long Name	SI Unit	Source
DCFGW(nuc)	DCF FROM INGEST. OF NUC (WATER)	[μSv Bq^{-1}]	Sampled
DCFGW(tot-Th)	DCF FROM INGEST. OF TH (WATER)	[μSv Bq^{-1}]	(4.1.4)
WATC(nuc,n)	CONCENTRATION OF RADIONUCLIDE IN WATER AT WATERSHED NODE N	[Bq m^{-3}]	3.3.6, 3.3.9
WATD(nuc,n)	INGEST. OF D.W. DOSE	[μSv a^{-1}]	4.1.4
WATIN	ANN. INTAKE OF WATER	[m^3 a^{-1}]	Sampled
WFLOC	FRAC. OF WATER LOCAL	[-]	Sampled
X232LA	ACTIV. FRACT. TH-232 IN SOLU. TH	[-]	1.3.1.7A

$$\text{DCFGW(tot-Th)} = 1.5 \times 10^{-1} + \text{X232LA} * (6.9 \times 10^{-1}) \qquad \text{(Table 13.2)}$$

$$\text{WATD(nuc,n)} = \text{DCFGW(nuc)} * \text{WATIN} * \text{WATC(n)} * \text{WFLOC} \qquad \text{(eqn. 13.4)}$$

Unit check:

DCFGW(tot-Th): not possible, no units given in Table 13.2.

WATD(nuc): [μSv Bq^{-1}] * [m^3 a^{-1}] * [Bq m^{-3}] * [-] = [μSv a^{-1}]

Note 1: For the average and critical receptors, WATIN and WFLOC are sampled from different distributions; see SENES Vol. 3, Tables 13.3 and 13.4.

Note 2: WATD is location-dependent, with "n" equivalent to a watershed node.

Note 3: For nuc = total thorium, DCFGW(nuc) is calculated as shown. For nuc = U, Ra and Pb, these are sampled (input) parameters.

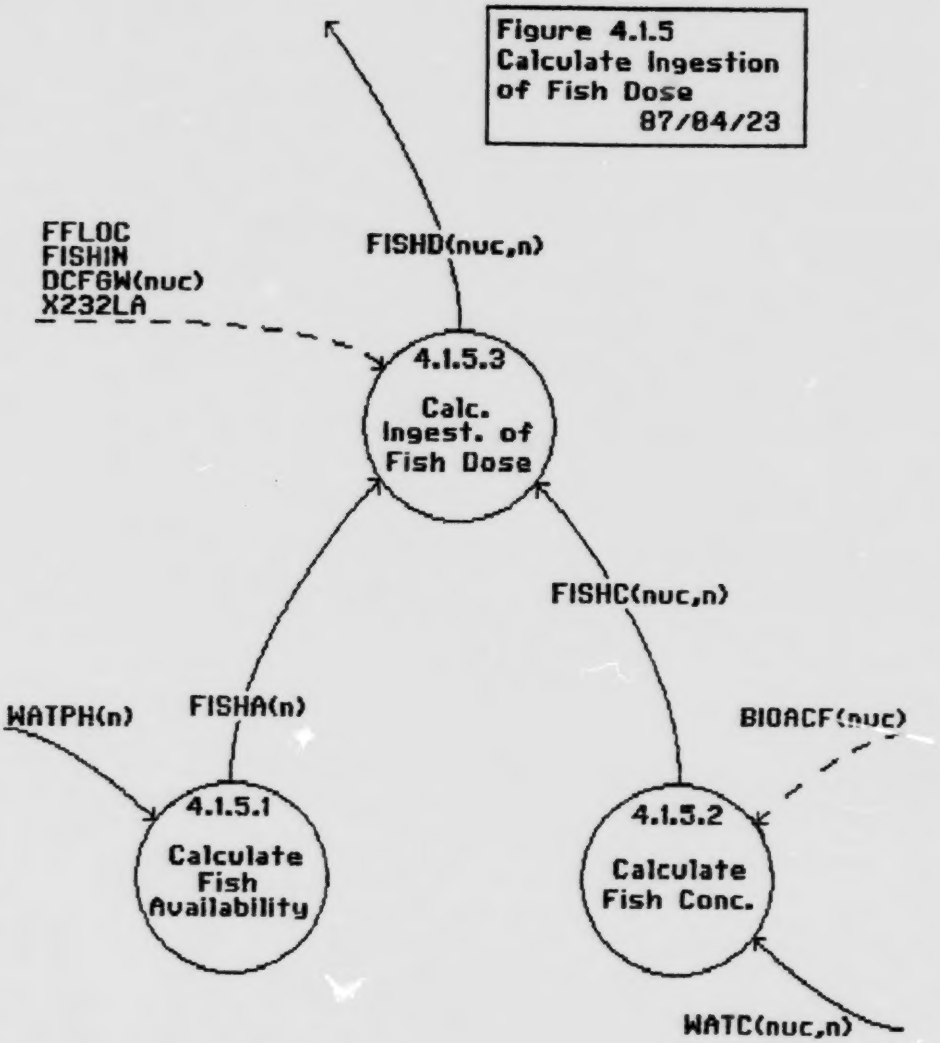


Figure 4.1.5
Calculate Ingestion
of Fish Dose
87/04/23

FISHD(nuc,n)
FFLOC
FISHIN
DCFGW(nuc)
X232LA
4.1.5.3
Calc.
Ingest. of
Fish Dose
FISHC(nuc,n)
FISHA(n)
WATPH(n)
BIOACF(nuc)
4.1.5.1
Calculate
Fish
Availability
4.1.5.2
Calculate
Fish Conc.
WATC(nuc,n)

Note: DCFGW(Th) is a calculated parameter.

Figure 4.1.5.1
Calculate FISH
AVAILABILITY
(FISHA(n))

FISHA(n) - FISH AVAILABILITY [-].
The fraction of fish available at the pH of the watershed at node "n" compared to the normal population of fish expected to be available if pH > 6.

$$\boxed{\text{FISHA(n)} \longleftarrow \text{WATPH(n)}}$$

Short Name	Long Name	SI Unit	Source
FISHA(n)	FISH AVAILABILITY	[-]	4.1.5.1
WATPH(n)	PH OF LAKE	[-]	3.2.7

If: $\text{WATPH(n)} > 6.0$ then $\text{FISHA(n)} = 1.0$

else if: $5.0 < \text{WATPH(n)} \leq 6.0$ then $\text{FISHA(n)} = 0.75 + 0.25 * (\text{WATPH(n)} - 5.0)$

else if: $4.5 < \text{WATPH(n)} \leq 5.0$ then $\text{FISHA(n)} = 0.25 + 1.0 * (\text{WATPH(n)} - 4.5)$

else if: $3.5 < \text{WATPH(n)} \leq 4.5$ then $\text{FISHA(n)} = 0.25 * (\text{WATPH(n)} - 3.5)$

else if: $\text{WATPH(n)} \leq 3.5$ then $\text{FISHA(n)} = 0.0$

(eqn. 11.1)

Unit check:

pH is dimensionless by definition and the constants in these equations are also assumed to be dimensionless.

FISHC(nuc,n) - FISH CONC. [Bq g^{-1}(wet)]. Concentration of the radionuclide "nuc" in game fish flesh (nuc = U-nat, Th-tot, Ra-226, Pb-210) at watershed node "n".

Figure 4.1.5.2
Calculate FISH CONC.

(FISHC(nuc,n))

$$\begin{tikzcd}
\text{BIOACF(nuc)} \arrow[r, dashed] & \text{FISHC(nuc,n)} & \text{WATC(nuc,n)} \arrow[l]
\end{tikzcd}$$

Short Name	Long Name	SI Unit	Source
BIOACF(nuc)	FISH BIOACCUM. FACTOR	[m^3 g^{-1}]	Sampled
FISHC(nuc,n)	FISH CONC.	[Bq g^{-1}]	4.1.5.2
WATC(nuc,n)	CONCENTRATION OF RADIONUCLIDE IN WATER AT WATERSHED NODE N	[Bq m^{-3}]	3.3.6, 3.3.9

$$\text{FISHC(nuc,n)} = \text{BIOACF(nuc)} * \text{WATC(nuc,n)} \qquad \text{(eqn. 11.2)}$$

Unit check:

$$[\text{Bq } g^{-1}(\text{wet}) \cdot \text{Bq}^{-1} \text{ m}^3] * [\text{Bq m}^{-3}]$$
$$= [\text{Bq } g^{-1}(\text{wet})]$$

Note: There is an inconsistency in units for FISHC(nuc,n) (= $[F_i]_{n,t}$) in eqn. (11.2), Table 11.5, eqn. (13.5) and Tables 13.3 and 13.4. The units shown have been assumed.

FISHD(nuc,n) - INGEST. OF FISH DOSE [µSv a^{-1}]. Average annual whole body dose of radionuclide "nuc" (nuc = nat-U, tot-Th, Ra-226, Pb-210) from ingestion of fish for a specific location (watershed node) and receptor type.

Figure 4.1.5.3
Calculate INGEST. OF
FISH DOSE
(FISHD(nuc,n))

```
DCFGW(tot-Th)
DCFGW(nuc)                                        FISHA(n)
FISHIN          - - ->  FISHD(nuc,n)  <——         FISHC(nuc,n)
FFLOC

X232LA          - - ->  DCFGW(tot-Th)
```

Short Name	Long Name	SI Unit	Source
DCFGW(nuc)	DCF FROM INGEST. OF NUC (WATER)	[µSv Bq^{-1}]	Sampled
DCFGW(tot-Th)	DCF FROM INGEST. OF TH (WATER)	[µSv Bq^{-1}]	(4.1.5.3)
FFLOC	FRAC. OF FISH LOCAL	[-]	Sampled
FISHA(n)	FISH AVAILABILITY	[-]	4.1.5.1
FISHC(nuc,n)	FISH CONC.	[Bq g^{-1}]	4.1.5.2
FISHD(nuc,n)	INGEST. OF FISH DOSE	[µSv a^{-1}]	4.1.5.3
FISHIN	ANN. INTAKE OF FISH	[g a^{-1}]	Sampled
X232LA	ACTIV. FRACT. TH-232 IN SOLU. TH	[-]	1.3.1.7A

$$\text{DCFGW(tot-Th)} = 1.5 \times 10^{-1} + \text{X232LA} * (6.9 \times 10^{-1}) \qquad \text{(Table 13.2)}$$

$$\text{FISHD(nuc,n)} = \text{DCFGW(nuc)} * \text{FISHIN} * \text{FISHC(nuc,n)} * \text{FFLOC} * \text{FISHA(n)} \qquad \text{(eqn. 13.5)}$$

Unit check:

DCFGW(tot-Th): not possible, no units given in Table 13.2.

FISHD(nuc): $[\mu Sv\ Bq^{-1}] * [g(wet)\ a^{-1}] * [Bq\ g^{-1}(wet) * [-] * [-] = [\mu Sv\ a^{-1}]$

Note 1: For the average receptor, FISHIN and FFLOC are sampled from different distributions; see SENES, Vol. 3, Tables 13.3 and 13.4.

Note 2: FISHD, FISHA and FISHC are location-dependent, and could be required at any of the 8 watershed nodes.

Note 3: For nuc = total Th, DCFGW(nuc) is calculated as shown. For nuc = U, Ra and Pb, these are sampled (input) parameters.

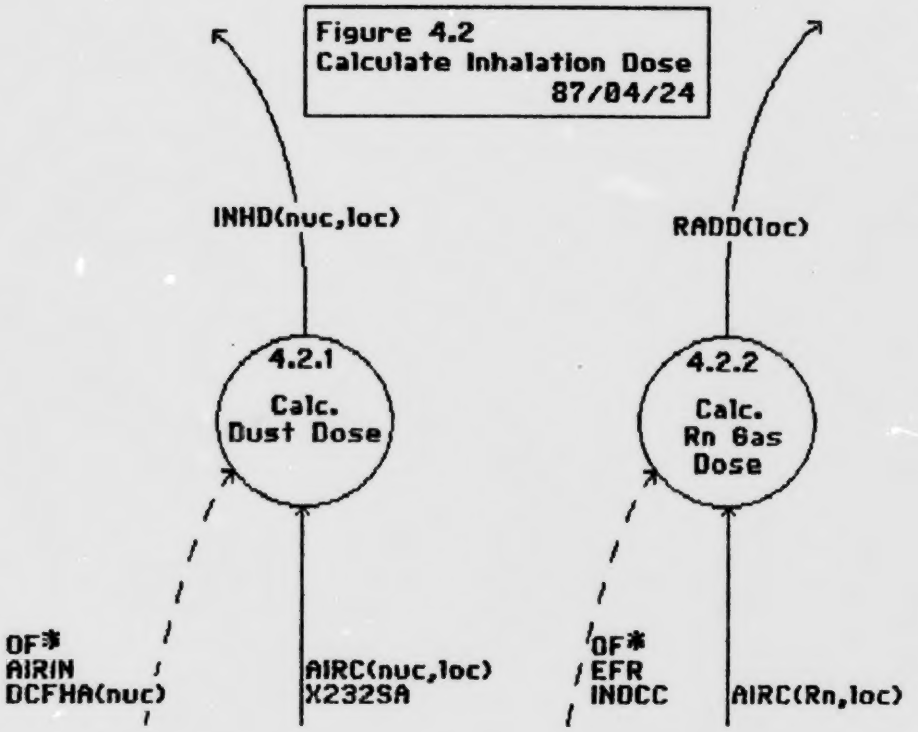


Figure 4.2
Calculate Inhalation Dose
87/04/24

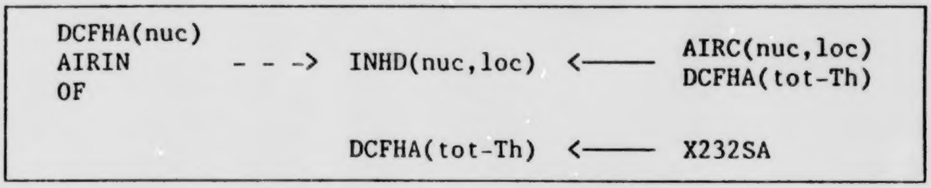
INHD(nuc,loc)
RADD(loc)
4.2.1
Calc.
Dust Dose
4.2.2
Calc.
Rn Gas
Dose
OF*
AIRIN
DCFHA(nuc)
AIRC(nuc,loc)
X232SA
OF*
EFR
INOCC
AIRC(Rn,loc)

Note: DCFHA(Th) is a time-dependent calculated parameter.

INHD(nuc,loc) - DUST DOSE [$\mu Sv\ a^{-1}$].
Average annual whole body dose of radionuclide "nuc" (nuc = U-nat, Th-tot, Ra-226, Pb-210) from inhalation of dust for a specific location and receptor type.

Figure 4.2.1
Calculate DUST DOSE

(INHD(nuc,loc))



Short Name	Long Name	SI Unit	Source
AIRC(nuc,loc)	CONC. OF CONTAMINANT (NUC) IN AIR AT RECEPTOR	[$Bq\ m^{-3}$]	2.3.5
AIRIN	ANN. INHAL. RATE	[$m^3\ a^{-1}$]	Sampled
DCFHA(nuc)	DCF FROM INHAL. OF NUC	[$\mu Sv\ Bq^{-1}$]	Sampled
DCFHA(tot-Th)	DCF FROM INHAL. OF TH	[$\mu Sv\ Bq^{-1}$]	(4.2.1)
INHD(nuc,loc)	DUST DOSE	[$\mu Sv\ a^{-1}$]	4.2.1
OF	OCCUPANCY FACTOR	[-]	Sampled
X232SA	ACT. FRACT. TH-232 IN SURF. SOLID TH	[-]	1.3.2.5C

DCFHA(tot-Th) = 7.0×10^1 + X232SA * (3.2×10^2) (page 13-5)

INHD(nuc,loc) = DCFHA(nuc) * AIRIN * AIRC(nuc,loc) * OF (eqn. 13.1; on page 13-15)

Unit check:

DCFHA(total Th): not possible; constants are not identified on page 13-5.

INHD: [$\mu Sv\ Bq^{-1}$] * [$m^3\ a^{-1}$] * [$Bq\ m^{-3}$] * [-]
= [$\mu Sv\ a^{-1}$]

Note 1: For the average receptor, AIRIN and OF are sampled from different distributions; see SENES Vol. 3, Tables 13.3 and 13.4.

Note 2: INHD(nuc,loc) and AIRC(nuc,loc) are location-dependent.

Note 3: DCFHA(total Th) is calculated using the equation shown. DCFHA(nuc), for nuc = U, Ra and Pb, are sampled (input) parameters.

Figure 4.2.2
Calculate RN GAS DOSE

(RADD(loc))

RADD(loc) - RN GAS DOSE [μSv a^{-1}].
Average annual whole body dose due to inhalation of radon and its daughter products for a specific location and receptor type.

OF
INOCC - - -> RADD(loc) <—— AIRC(Rn,loc)
EFR

Short Name	Long Name	SI Unit	Source
AIRC(Rn,loc)	CONC. OF CONTAMINANT (RN-222) IN AIR AT RECEPTOR	[Bq m^{-3}]	2.3.5
EFR	EQUIL. FACTOR FOR RN	[-]	Sampled
INOCC	FRAC. OUTDOORS	[-]	Sampled
OF	OCCUPANCY FACTOR	[-]	Sampled
RADD(loc)	RN GAS DOSE	[μSv a^{-1}]	4.2.2

$$RADD(loc) = AIRC(Rn,loc) * OF * INOCC * EFR * 69.6$$

(eqn. on page 13-17;
see Note 4)

Unit check:

$$[Bq\ m^{-3}] * [-] * [-] * [-] * [\mu Sv\ Bq^{-1}\ m^{3}\ a^{-1}]$$
$$= [\mu Sv\ a^{-1}]$$

Note 1: The constant 69.6 is discussed on page 13-17 and is given the units indicated. See also Note 4.

Note 2: For the average receptor, OF is sampled from a different distribution; see SENES Vol. 3, Tables 13.3 and 13.4. INOCC was chosen to be independent of receptor type; see SENES, p. 13-18.

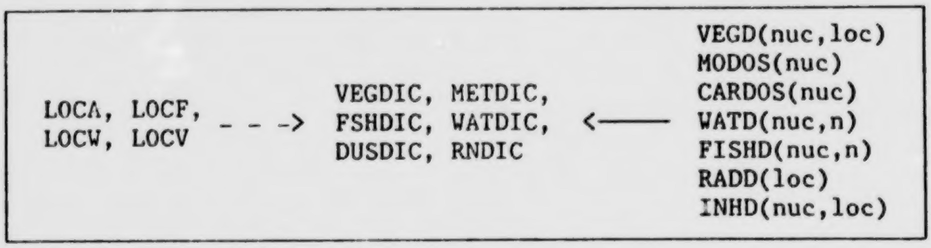
Note 3: RADD(loc) and AIRC(Rn,loc) are location-dependent.

Note 4: Inspection of the UTAP2 code shows that the value 69.6 has been used instead of the value 6.96 which is given in the SENES report (see page 13-17). Calculation of this factor, based on the data on page 13-17, confirms that the value 69.6 is (probably) correct. The value 69.6 has been used in SYVAC3-UT2 (BWG, 87-04-10).

Figure 4.3
Calculate INTERNAL DOSES (VEGDIC, METDIC, FSHDIC, WATDIC, DUSDIC, RNDIC)
(Page 1 of 2)

VEGDIC(METDIC,FSHDIC,WATDIC) - INTERNAL DOSE (CR) FROM VEGETABLES (MEAT, FISH, WATER) [μSv a^{-1}]. Internal dose to a critical receptor due to ingestion of contaminated vegetables (meat, fish, water).

DUSDIC(RNDIC) - INTERNAL DOSE (CR) FROM DUST (RADON) [μSv a^{-1}]. Internal dose to a critical receptor due to inhalation of contaminants in dust (of radon and its daughters).



Short Name	Long Name	SI Unit	Source
CARDOS(nuc)	INGEST. OF CARIBOU DOSE	[μSv a^{-1}]	4.1.3
DUSDIC	INTERNAL DOSES FROM DUST	[μSv a^{-1}]	4.3
FISHD(nuc,n)	INGEST. OF FISH DOSE	[μSv a^{-1}]	4.1.5
FSHDIC	INTERNAL DOSES FROM FISH	[μSv a^{-1}]	4.3
INHD(nuc,loc)	DUST DOSE	[μSv a^{-1}]	4.2.1
LOCA	LOCATION OF RECEPTOR'S AIR	[-]	Sampled
LOCF	LOCATION OF RECEPTOR'S FISH	[-]	Sampled
LOCV	LOCATION OF RECEPTOR'S VEGETABLES	[-]	Sampled
LOCW	LOCATION OF RECEPTOR'S WATER	[-]	Sampled
METDIC	INTERNAL DOSES FROM MEAT	[μSv a^{-1}]	4.3
MODOS(nuc)	INGEST. OF MOOSE DOSE	[μSv a^{-1}]	4.1.2
RADD(loc)	RN GAS DOSE	[μSv a^{-1}]	4.2.2
RNDIC	INTERNAL DOSES FROM RADON	[μSv a^{-1}]	4.3
VEGD(nuc,loc)	INGEST. OF VEG. DOSE	[μSv a^{-1}]	4.1.1
VEGDIC	INTERNAL DOSES FROM VEGETABLES	[μSv a^{-1}]	4.3
WATD(nuc,n)	INGEST. OF D.W. DOSE	[μSv a^{-1}]	4.1.4
WATDIC	INTERNAL DOSES FROM WATER	[μSv a^{-1}]	4.3

$$\mathrm{METDIC} = \sum_{nuc} (\mathrm{MODOS(nuc)} + \mathrm{CARDOS(nuc)})$$

$$\mathrm{VEGDIC} = \sum_{nuc} \mathrm{VEGD(nuc,LOCV)}$$

(See Note 1)

$$\mathrm{FSHDIC} = \sum_{nuc} \mathrm{FISHD(nuc,LOCF)}$$

$$\mathrm{WATDIC} = \sum_{nuc} \mathrm{WATD(nuc,LOCW)}$$

$$\mathrm{DUSDIC} = \sum_{nuc} \mathrm{INHD(nuc,LOCA)}$$

$$\mathrm{RNDIC} = \mathrm{RADD(LOCA)}$$

Figure 4.3
Calculate INTERNAL DOSES
(VEGDIC, METDIC, FSHDIC,
WATDIC, DUSDIC, RNDIC)
(Page 2 of 2)

Unit check:
All quantities are in [μSv a^{-1}].

Note 1: No equations are given in SENES Vol. 3 for these calculations. nuc = nat U, tot Th, Ra-226 and Pb-210. (BWG)

Note 2: loc = ring and sector location ($1 \leq loc \leq 80$) relating to the critical receptor. LOCA and LOCV are input location parameters that are, in general, different.

Note 3: n = watershed node location ($1 \leq n \leq 8$) relating to the critical receptor. LOCF and LOCW are input location parameters that are, in general, different.

Note 4: This figure, and other figures in this set, are for a critical receptor. An identical figure would apply for the internal doses for an average receptor: VEGDIA, METDIA, FSHDIA, WATDIA, DUSDIA and RNDIA. The location parameters LOCA, LOCF, LOCF and LOCW are, in general, different for the critical and average receptors.

Figure 4.4
Calculate TOTAL INTERNAL DOSE (DOSEIC)

DOSEIC - TOTAL INTERNAL DOSE (CR) [μSv a^{-1}].
Total internal dose to a critical receptor due to the ingestion of contaminated vegetables, caribou, moose, fish and drinking water, and due to the inhalation of contaminants in dust and radon and its daughters.

$$\boxed{\text{DOSEIC} \longleftarrow \begin{matrix}\text{VEGDIC, METDIC, FSHDIC,}\\ \text{WATDIC, DUSDIC, RNDIC}\end{matrix}}$$

Short Name	Long Name	SI Unit	Source
DOSEIC	TOTAL INTERNAL DOSE	[μSv a^{-1}]	4.4
DUSDIC	INTERNAL DOSES FROM DUST	[μSv a^{-1}]	4.3
FSHDIC	INTERNAL DOSES FROM FISH	[μSv a^{-1}]	4.3
METDIC	INTERNAL DOSES FROM MEAT	[μSv a^{-1}]	4.3
RNDIC	INTERNAL DOSES FROM RADON	[μSv a^{-1}]	4.3
VEGDIC	INTERNAL DOSES FROM VEGETABLES	[μSv a^{-1}]	4.3
WATDIC	INTERNAL DOSES FROM WATER	[μSv a^{-1}]	4.3

$$\text{DOSEIC} = \text{VEGDIC} + \text{METDIC} + \text{FSHDIC} + \text{WATDIC} + \text{DUSDIC} + \text{RNDIC}$$

(see Note)

Unit check:
All quantities are in [μSv a^{-1}].

Note: No equation is provided in SENES Vol. 3 (BWG). An equivalent equation applies (presumably) to the average receptor, involving the variables DOSEIA, VEGDIA, METDIA, FSHDIA, WATDIA, DUSDIA and RNDIA.

APPENDIX C: DATA DICTIONARY FOR THE TAILINGS MODEL

Specifications for the UTAP (Uranium Tailings Assessment Program) model have been developed from the SENES Phase III Report.[1] The specifications consist of three components: data flow diagrams (DFD's), minispecifications (minispecs), and the data dictionary (DD). The following notes describe the format of the data dictionary, and is followed by the data dictionary developed from the uranium tailings model. Notes for the DFD's and minispecs are presented in Appendix B.

Data dictionary

The data dictionary is an alphabetical list of all variables and key words used in the specifications. The following fields are presented for each variable:

(1) Short name: Every variable has a short name of at most six characters that can be used as a FORTRAN variable name. This appears first and is used for alphabetical ordering of the data dictionary.

(2) Long name: Every variable also has a long name consisting of several words, often abbreviated, to be used in formal references to the variable, such as in the data flow diagrams and minispecs.

(3) SI units: Metric units are provided for every variable. They appear inside square brackets (e.g. [mol s^{-1}]). Where no units apply, "[-]" is used.

(4) Definition: Each variable is defined in one or two sentences that explain what physical quantity the variable represents. The definition states if the variable depends on time or space variables, or is specific to one nuclide. It contains all the relevant information from SENES documentation.

(5) Background information: The data dictionary states where every variable was generated and used in the originating documentation, what problems have arisen in using the documentation related to that variable, and what consequent corrections have been made.

(6) Sampled/calculated: The data dictionary states whether a variable is an input (sampled) parameter or a calculated parameter. If the variable is a sampled parameter, the input data (including probability distribution data) is listed. If the variable is calculated, the appropriate equation is referenced.

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[1] SENES, 1986. Probabilistic Model Development for the Assessment of the Long-Term Effects of Uranium Mill Tailings in Canada - Phase III; Volume 3 - Uranium Tailings Assessment Program (UTAP) Component Model Documentation. Contract report prepared under contract # 0SQ85-00182 for the National Uranium Tailings Program, Canada Centre for Mineral and Energy Technology, Energy, Mines and Resources Canada, 555 Booth Street, Ottawa, Ontario, K1A 0G1.

(7) Equation: Where a variable is calculated according to a simple equation, that equation also appears in the data dictionary.

In addition to definitions of variables, the data dictionary also contains definitions of key words like "MODULE" and "UNSAT. ZONE" that appear frequently and have a specific meaning.

DATA DICTIONARY FOR THE NUTP TAILINGS SUBMODEL
(1987-Feb-06)

A11,A21 MATRIX PARAMETERS USED IN WATEX [Bq a^{-1}]. Intermediate parameters used in the calculation of WATRW and WATRS in the WATEX module. These time dependent parameters are defined in equations below equations (10.32) and (10.33) in SENES Vol. 3.

A12,A13,A22,A23 MATRIX PARAMETERS USED IN WATEX [a^{-1}]. Intermediate parameters used in the calculation of WATRW and WATRS in the WATEX module. These time dependent parameters are defined in equations near equations (10.32) and (10.33) in SENES Vol. 3.

AA(nuc,n) AA PARAMETER USED IN WATEX [Bq]. Intermediate parameter used in the calculation of WATRW and WATRS in the WATEX module. This time dependent parameter is defined in an equation at the top of page 10-29 in SENES Vol. 3.

ACARC(nuc) AIR - CARIBOU CONC. [Bq g^{-1}(wet)]. Concentration of the radionuclide "nuc" in caribou flesh due to the air pathway (nuc = U-nat, Th-tot, Ra-226, Pb-210). Time dependent parameter used in the DOSE module and calculated from equation (12.1) of SENES Vol. 3.

ACTCO ACTIVITY COEFFICIENT IN LAKE [-]. Activity coefficient for divalent ions used in the lake pH calculations, where the ionic strength is relatively low. Used in the LAKEPH module. ACTCO is sampled from the following distribution:
Triangular (0.6, 0.8, 0.9)

AEXPT EXPOSED TAILINGS SURFACE AREA [m^2]. Exposed surface area of the tailings, as a function of time. AEXPT is used in DUST module. It is calculated (from the definition of FVEG) for tailings partially covered with vegetation using the equation:
AEXPT = (1.0 - FVEG) x ATAIL
This was confirmed by SENES (letter 1986-10-15), but not explicitly given in the final version of SENES Vol. 3. The vegetation fraction, FVEG, is calculated in EROS (part of SENES SOURCE), but AEXPT is not in the table of model variables for that module. However, the DUST module describes AEXPT as calculated in SOURCE (Table 4.3), and we have calculated it in the EROS module.

AFACT FRAC. OF ACTIVITY IN VEG. TYPE A [-]. The fraction of activity remaining in above (A) ground vegetables after preparation as food. Input parameter used in the DOSE module and sampled from:
Uniform (0.5,1.0)

AFLOC FRAC. OF VEG. TYPE A LOCALLY GROWN [-]. The fraction of above (A) ground vegetables used as food that is grown locally. Receptor specific input parameter used in the DOSE module and sampled from:
Triangular (0.1,0.3,0.6) - critical receptor
Triangular (0.0,0.1,0.2) - average receptor

AIRC(nuc,loc)	CONC. OF CONTAMINANT IN AIR AT RECEPTOR [Bq m^{-3}]. Average annual concentration of radionuclide (nuc = U-nat, Th-tot, Ra-226, Pb-210, Rn-222) associated with dust (or gas) in air at a receptor (vegetables and vegetation and/or a 'critical' or 'average' man), (loc=1,82). Time dependent variable calculated in the AIRDIS module and used in the SOIL, DOSE and VEGCON modules. Calculated for the eighty sector/range locations (1,80) using equation (5.1) of SENES Vol. 3. Summation over the terms for the separate stability classes has been assumed for each location to obtain AIRC, although this is not clear from equation (5.1). Calculated for the watershed (loc=82) and total study area (loc=81) by taking the average over the appropriate locations. Watershed area locations were specified in a letter from SENES (1986-12-11). NOTE: See also DDDs 2.3.5 to 2.3.7A for modifications to the equations for AIRC.
AIRDIS	MODULE. All processes required to calculate concentrations in air at the receptor, given source concentrations at the tailings source (see DFD 2 and DDD 2.3). The major outputs from AIRDIS are AIRC(nuc), (nuc=Pb-210, Ra-226, Rn, tot-Th, nat-U).
AIRIN	ANN. INHAL. RATE [m^3 a^{-1}]. The average annual inhalation rate of the individual. Input receptor specific parameter used in the DOSE module and sampled from: Constant (8.4 x 10^3). The same value was used for critical and average receptors.
ALDIS	LONGITUDIAL DISPERSIVITY [m]. Dispersivity used as a measure of the solid phase to cause mechanical dispersion. Variable calculated in the GWATER module from equation 9.19 of SENES Vol. 3.
AMOC(nuc)	AIR - MOOSE CONC. [Bq g^{-1}(wet)]. Concentration of the radionuclide "nuc" in moose flesh due to the air pathway (nuc = U-nat, Th-tot, Ra-226, Pb-210). Time dependent parameter used in the DOSE module and calculated from equation (12.3) of SENES Vol. 3.
APBI	INIT. ACTIV. PB-210 IN TAILINGS [Bq g^{-1}]. Initial solid phase activity of Pb-210 in the tailings. Intermediate parameter used in the TSOURC modules and calculated from equations (3.7.33) and (3.7.45) of SENES Vol. 3.
AQVEGC(nuc)	CONC. IN MOOSE AQUATIC FOODS [Bq g^{-1}(wet)]. The concentration of radionuclide "nuc" (nuc = U-nat, Th-tot, Ra-226, Pb-210) in aquatic vegetation consumed by moose. Intermediate time dependent parameter used in the DOSE module and calculated using equation (11.3) of SENES Vol. 3.
ARADI	INIT. ACTIV. RA-226 IN TAILINGS [Bq g^{-1}]. Initial solid phase activity of Ra-226 in the tailings. Intermediate parameter used in the TSOURC modules and calculated from equation (3.7.33) of SENES Vol. 3.
AT230I	INIT. ACTIV. TH-230 IN TAILINGS [Bq g^{-1}]. The initial activity of (solid) Th-230 in the tailings. Intermediate parameter calculated in the TSOURC modules using equation (3.7.13) of SENES Vol. 3.
ATAIL	INITIAL EXPOSED TAILINGS SURFACE AREA [m^2]. Initial exposed surface area of the tailings. ATAIL is a sampled (input) parameter used in the TSOURC, EROS, RADON, AIRDIS and GWATER modules. It is also used in the LAKEPH module in the calculation of SFLOW. It is sampled from: Constant (5 x 10^5)
AU2380	INITIAL ACTIVITY U-238 IN ORE [Bq g^{-1}]. The initial activity due to uranium-238 in the ore before processing. Intermediate para-

meter used in the TSOURC modules and calculated using equation (3.7.2) of SENES Vol. 3.

AUNATO INITIAL ACTIVITY OF U-NAT IN ORE [Bq g^{-1}]. The initial activity due to natural uranium in the ore before processing. Intermediate parameter used in the TSOURC modules and calculated using equation (3.7.1) of SENES Vol. 3.

AUNATT INITIAL ACTIVITY OF U-NAT IN TAILINGS [Bq g^{-1}]. The initial activity due to natural uranium in the tailings. Intermediate parameter used in the TSOURC modules and calculated using equation (3.7.3) of SENES Vol. 3.

AVEGC(nuc,loc) CONC. OF RADIONUCLIDE IN ABOVE-GROUND VEGETABLES [Bq g^{-1}(wet weight)]. Average annual concentration of radionuclide (nuc) in above-ground vegetables due to foliar retention of the radionuclide deposited from dust in the air and to root uptake. Values are calculated as a function of time and location. Variable calculated in the VEGCON module and used in the DOSE module. Calculated using equation (8.1) of SENES Vol. 3.
NOTE: Identical to CVEG(nuc,1,loc), where CVEG has been used to generalize the calculations for different vegetation types.

AVEGIN AV. INTAKE OF VEG. TYPE A [g(wet) a^{-1}]. The average annual intake of above (A) ground vegetables. Receptor specific input parameter used in the DOSE module and sampled from:
Constant (1.57 x 10^5) - critical receptor
Constant (3.99 x 10^4) - average receptor

AVPRCP AVERAGE NET PRECIPITATION [m a^{-1}]. The long-term annual precipitation used to calculate the volumetric seepage rate through the the tailings and into the aquifer. Used in the TSOURC and GWATER modules and sampled from:
Constant (0.4)

AW(RNGMID(dis),st) VERTICAL DISPERSION LINEAR PARAMETER [m]. Parameter "a" in the equation to calculate the vertical dispersion coefficient for different stability classes (st) and distances.. Used in the AIRDIS module equation 5.6. Sampled from:

Stability Class	500 < RNGMID <5000	5000 < RNGMID < 50000
A	0.0002539	0.0002539
B	0.04936	0.04936
C	0.1014	0.1154
D	0.2591	0.7368
E & F	0.2017	1.5763

Values for the parameters are given in Table 5.2 of SENES Vol. 3. Units [m] have been assumed to permit a proper unit check.

AXGWAT CROSS-SECTIONAL AREA OF FLOW [m^2]. Cross-sectional area of the aquifer window. Input parameter used in the GWATER module and sampled from:
Constant (1000)

BASATI INIT. RA ASSOC. BA UNSAT. PLUS MIX [mol m^{-2}]. The initial total radium associated with $BaSO_4$ in the unsaturated and mixing zones of the tailings. Intermediate parameter used in the TSOURC modules, and calculated using equation (3.7.39) of SENES Vol. 3.

BB(nuc,n) BB PARAMETER USED IN WATEX [Bq]. Intermediate parameter used in the calculation of WATRW and WATRS in the WATEX module. This time dependent parameter is defined in an equation near the top of page 10-29 in SENES Vol. 3.

BED(eseg) BEDLOAD FOR SEGMENT [lb ft^{-1} a^{-1}]. The bedload contribution to erosion for segment "eseg" of the tailings pile. Intermediate time

dependent parameter used in the EROS module. Not explicitly defined in SENES Vol. 3, but calculated from an equation provided (letter, 1987-01-27) as a modification of the equation below equation (3.14.20).
NOTE: See DDD 1.6.3.7 for more complete comments.

BETA PYRITE OXIDATION FACTOR [mol m^{-3}]. Number of moles of pyrite oxidized per unit volume between TIME=t-Δt and TIME=t. Intermediate parameter used in the TSOURC modules and defined in an equation below equation (3.3.22) of SENES Vol. 3 (see also equation (3.8.1)).

BETAO(nuc,sla,loc) RADIONUCLIDE INPUT FOR SOIL LAYER [Bq a^{-1}]. Input rate to a soil layer (sla=1,NLAYER) of activity from a radionuclide, (nuc) (nuc= Ra-226, Pb-210, tot-Th, nat-U) at a receptor site (loc, loc=1,80). Intermediate parameter calculated in the SOIL module. Calculated for the surface soil layer using a modification of equation (6.11) of SENES Vol. 3:
BETAO(nuc,1,loc) = AIRC(nuc,loc) x DEPVEL x SOILA X SYEAR.
Calculated using equation (6.12) for the other soil layers.
NOTE: The factor SYEAR has been introduced in equation (6.11) to give BETAO in [Bq a^{-1}] rather than [Bq s^{-1}]
NOTE: See DDDs 2.4.1 and 2.4.5 for additional comments.

BETAI(nuc,sla,loc(?)) LEACHING LOSS RATE CONSTANT [a^{-1}] The rate constant for the loss of an element (nuc) (nuc= Ra, Pb, Th, U) from a soil layer (sla) by leaching. Intermediate parameter calculated in the SOIL module from equation 6.9 of SENES Vol. 3
NOTE: It is not clear if the value is location dependent. If Kd is sampled for each nuclide independently at each location then BETAI is also location dependent.
NOTE: See also DDD 2.4.2 for modifications to the equations for calculation of BETAI.

BEXP EXPONENT IN BEDLOAD EQN. [-]. An empirical exponent used in the bedload transport capacity equation. A parameter used in the EROS module and calculated from equation (3.14.11) of SENES Vol. 3. The limits for the expressions in equation (3.14.11) were modified according to a letter from SENES (1987-01-27).
NOTE: See DDD 1.6.1.6 for additional comments.

BFACT FRAC. OF ACTIVITY IN VEG. TYPE B [-]. The fraction of activity remaining in below (B) ground vegetables after preparation as food. Input parameter used in the DOSE module and sampled from:
Uniform (0.5,1.0)

BFLOC FRAC. OF VEG. TYPE B LOCALLY GROWN [-]. The fraction of below (B) ground vegetables used as food that is grown locally. Receptor specific input parameter used in the DOSE module and sampled from:
Triangular (0.1,0.3,0.6) - critical receptor
Triangular (0.0,0.1,0.2) - average receptor

BGW(nuc) B PARAMETER [m^{-1}]. Intermediate B parameter used in the calculation of groundwater radionuclide concentrations in GWATER (nuc = nat-U, tot-Th, Ra-226, Pb-210). Used in the GWATER module and calculated using an equation near equation 9.12 in SENES Vol. 3.

BIOACF(nuc) FISH BIOACCUM. FACTOR [Bq g^{-1}(wet) Bq^{-1} m^3]. The water-to-game fish flesh bioaccumulation factor for nuclide "nuc" (nuc = nat-U, tot-Th, Pb-210 and Ra-226). Input parameter used in the DOSE module and sampled from:

Lognormal (1.55×10^{-6}, 6.1, 1.0×10^{-8}, 5.8×10^{-5}) nuc = U-nat
(1.18×10^{-5}, 2.6, 1.1×10^{-6}, 1.1×10^{-4}) nuc = Th-tot
(1.31×10^{-5}, 3.3, 1.2×10^{-6}, 6.0×10^{-4}) nuc = Ra-226
(1.74×10^{-5}, 3.25, 1.7×10^{-6}, 5.7×10^{-4}) nuc = Pb-210

BRWSC(nuc) CONC. OF RADIONUCLIDE IN BROWSE VEGETATION [Bq g^{-1}(wet weight)]. Average annual concentration of radionuclide (nuc) in browse vegetation due to foliar retention of the radionuclide deposited from dust in the air and to root uptake. Values are calculated as a function of time and location. Variable calculated in the VEGCON module and used in the DOSE module. Calculated using equation (8.1) of SENES Vol. 3.
NOTE: Identical to CVEG(nuc,4,loc), where CVEG has been used to generalize the calculations for different vegetation types.

BSOIL SOIL STRUCT. CODE [-]. Soil structure code used in soil classification. Input parameter used in the EROS module and sampled from:
Constant (2.0)
(SENES letter, 1986-12-02).

BURYF FRACTION TO DEEP SEDIMENT [-]. The fraction of sedimenting material removed to the deep sediments. Input parameter used in the WATEX module and sampled from:
Uniform (0.5, 0.7)

BVEGC(nuc,loc) CONC. OF RADIONUCLIDE IN BELOW-GROUND VEGETABLES [Bq g^{-1}(wet weight)]. Average annual concentration of radionuclide (nuc) in below-ground vegetables due to foliar retention of the radionuclide deposited from dust in the air and to root uptake. Values are calculated as a function of time and location. Variable calculated in the VEGCON module and used in the DOSE module. Calculated using equation (8.1) of SENES Vol. 3.
NOTE: Identical to CVEG(nuc,2,loc), where CVEG has been used to generalize the calculations for different vegetation types.

BVEGIN AV. INTAKE OF VEG. TYPE B [g(wet) a^{-1}]. The average annual intake of below (B) ground vegetables. Receptor specific input parameter used in the DOSE module and sampled from:
Constant (7.0×10^{4}) - critical receptor
Constant (6.54×10^{4}) - average receptor

BW(RNGMID(dis),st) VERTICAL DISPERSION EXPONENT PARAMETER [-]. Exponent "b" in the equation to calculate the vertical dispersion coefficient for different stability classes (st) and distances. Used in the AIRDIS module equation 5.6.

Stability Class	500 < RNGMID <5000	5000 < RNGMID < 50000
A	2.0886 *	2.0886
B	1.1137	1.1137
C	0.9260	0.9109
D	0.6869	0.5642
E & F	0.6020	0.3606

Values for the parameters are given in Table 5.2 of SENES Vol. 3. The two values for stability class A are not identical in SENES Table 5.2, the value marked * being given as 2.086. They should be the same. The value given here is probably the correct value because it can be correctly rounded to give the value (2.089) noted in an earlier SENES draft. Units [-] have been assumed to permit a proper unit check.
NOTE: the values for classes A and B were rounded to four digits in the SENES code (BWG, 87-04-06).

CALIME	CA FROM CACO3 DISS. [mol m^{-3}]. Average solution concentration of calcium at the bottom of the unsaturated layer, between TIME=t-Δt and TIME=t and attributable to dissolution of $CaCO_3$. Used in the TSOURC modules and calculated using equation (3.3.68) of SENES Vol. 3 if gypsum is still present in the unsaturated layer, and equation (3.3.69) if all the gypsum has been leached from the unsaturated layer. CALIME is zero by definition if LIMEIN = 0.0.
CARDOS(nuc)	CARIBOU DOSE [μSv a^{-1}]. Average annual whole body dose of radionuclide "nuc" (nuc = nat-U, tot-Th, Ra-226, Pb-210) from ingestion of caribou meat for a specific location and receptor type. Intermediate time dependent parameter used in the DOSE module and calculated using equation (13.2) of SENES Vol. 3.
CARMIN	ANN. INTAKE OF CARIBOU [g(wet) a^{-1}]. The average annual intake of caribou meat. Receptor specific input parameter used in the DOSE module and sampled from: Constant (3.95 X 10^4) - critical receptor Uniform (0.0,3.2 X 10^3) - average receptor
CBAR	TOTAL BA CONC. BOTTOM UNSAT. ZONE [mol m^{-3}]. Total concentration of dissolved barium at the bottom of the unsaturated zone. Intermediate time dependent variable used in the TSOURC modules and calculated using equation (3.10.9) of SENES Vol. 3.
CBARI	INIT. SOLID CONC. BASO4 [mol m^{-3}]. The initial solid phase concentration of barium sulphate in the tailings. Intermediate parameter used in the TSOURC modules and calculated using equations (3.7.36) and (3.7.38) of SENES Vol. 3.
CFFM	CONVERSION FACTOR FEET TO METRES [m ft^{-1}]. The factor used to convert lengths from units of metres to units of feet. Used in the EROS module, but not explicitly given by SENES. A value has been provided in a letter (1987-01-13). Sampled from: Constant (0.3048).
CFLOC	FRAC. OF CAR. LOCAL [-]. The fraction of the annual intake of caribou meat that is from local caribou. Receptor specific input parameter used in the DOSE module and sampled from: Uniform (0.0,1.0) for both critical and average receptors. NOTE: CARLOC has been used in our DDD's.
CIGPB	CONCENTRATION PB-210 GROWN-IN FROM RA-226 [Bq m^{-3}]. The concentration of Pb-210 at the discharge point resulting from the decay of Ra-226. Intermediate variable used in the GWATER module and calculated using equations 9.8a and 9.8b of SENES Vol. 3.
CLEAD	TOTAL AQ. PB CONC. BOTTOM UNSAT. ZONE [mol m^{-3}]. Total concentration of dissolved lead at the bottom of the unsaturated zone. Intermediate time dependent variable used in the TSOURC modules and calculated using equation (3.11.1) of SENES Vol. 3.
CLEADI	INITIAL CONC. PB [mol m^{-3}]. The initial concentration of $PbSO_4$ in the tailings. Input parameter used in the TSOURC modules and sampled from: Triangular (1.0, 2.0, 3.0)
CONC(1,1,1)	INIT. CONC. U IN TAILINGS SOLID [Bq m^{-3}]. Initial concentration of natural uranium in the solid phase of the tailings. Intermediate variable used in the TSOURC modules. Calculated using equation (3.7.4) of SENES Vol. 3.
CONC(1,1,3)	CONC. SOLID U IN UNSAT. ZONE [Bq m^{-3}]. Solid phase concentration of uranium in the unsaturated zone. Major time dependent output from the TSOURC modules; used in the WATEX and DUST modules. Calculated using modifications of equations (3.8.2) and (3.8.3) of

SENES Vol. 3; Units are converted to [Bq m^{-3}] using UCF.
NOTE: At t=0, CONC(1,1,3) = CONC(1,1,1) (inspection of the UTAP2 code).

CONC(2,1,3) TOTAL TH IN SOLID PHASE, UNSAT. ZONE [Bq m^{-3}]. Concentration of total thorium in the solid phase of the unsaturated zone. Major time dependent output from the TSOURC modules; used in the WATEX and DUST modules. Calculated using equation (3.9.10) of SENES Vol. 3.

CONC(3,1,3) CONC. SOLID PB-210 IN LAYER 1 [Bq m^{-3}]. Solid phase concentration of lead-210 in the upper layer of the unsaturated zone. Major time dependent output from the TSOURC modules; used in the WATEX and DUST modules. Calculated using equation (3.11.8) of SENES Vol. 3, modified by the introduction of the factor PBCF to convert the concentration to [Bq m^{-3}]
NOTE: units given as [mol m^{-3}] at equation (3.11.8) of SENES Vol. 3.

CONC(4,1,3) CONC. SOLID RA IN LAYER 1 [Bq m^{-3}]. Solid phase concentration of radium in the upper layer of the unsaturated zone. Major time dependent output from the TSOURC modules; used in the WATEX, DUST and RADON modules. Calculated using equation (3.10.24) of SENES Vol. 3, modified by the introduction of the factor RACF to convert the radium concentration to [Bq m^{-3}].
NOTE: At TIME=0, CONC(4,1,3) = CRADTI * RACF (inspection of the UTAP2 code).
NOTE: units given as [mol m^{-3}] at equation (3.10.24) of SENES Vol. 3.

CONC(4,2,3) CONC. SOLID RA IN LAYER 2 [Bq m^{-3}]. Solid phase concentration of radium in the lower layer of the unsaturated zone. Major time dependent output from the TSOURC modules; used in the RADON module. Calculated using equation (3.10.25) of SENES Vol. 3, modified to give units of [Bq m^{-3}] as in Table A.3 of SENES Vol. 3.
NOTE: At TIME=0, CONC(4,2,3) = CRADI * RACF (inspection of the UTAP2 code).

CONC(nuc,1,3) see CONC(1,1,3), CONC(2,1,3), CONC(3,1,3), CONC(4,1,3) for nuc = nat-U, tot-Th, Ra-226, Pb-210, respectively.

CONC(nuc,j,2), (nuc=1-4, j=1-4) as for CONC(nuc,j,3) but for time = t-Δt.

CPBI INIT. SOLID PHASE CONC. PB-210 IN TAILINGS [mol m^{-3}]. The initial solid phase concentration of Pb-210 in the tailings. Used in the TSOURC modules and calculated from equation (3.7.47) of SENES Vol. 3.

CPBIN NOTE: SENES uses CPBIN to refer to the lead-210 inputs either to layer 3 (SENES $[Pb_{in}]$, our CPBIN3) or to layer 4 (SENES $[Pb_{in,4}]$, our CPBIN4).

CPBIN3 CONC. PB-210 MIXING ZONE INPUTS [mol m^{-3}]. The concentration of lead-210 resulting from the various inputs to the mixing layer of the saturated zone. Time dependent intermediate parameter used in the TSOURC modules, and calculated using equations (3.11.14), (3.11.15) and (3.11.16) of SENES Vol. 3. The initial condition is specified by use of equation (3.11.15) for the time interval between TIME=-Δt and TIME=0. Equation (3.7.53) is not used for layer 3 (SENES letter, 1987-01-27).
NOTE: SENES uses CPBIN to refer to either the inputs to layer 3 (our CPBIN3) or to layer 4 (our CPBIN4).

CPBIN4 CONC. PB-210 BOTTOM LAYER INPUTS [mol m^{-3}]. The concentration of lead-210 resulting from the various inputs to the bottom layer of

	the saturated zone. Time dependent intermediate parameter used in the TSOURC modules, and calculated using equations (3.11.20) and (3.11.21) of SENES Vol. 3. The initial condition is specified by use of equation (3.11.21) for the time interval between TIME=-Δt and TIME=0. Equation (3.7.53) is not used for layer 4 (SENES letter, 1987-01-27). NOTE: SENES uses CPBIN to refer to either the inputs to layer 3 (our CPBIN3) or to layer 4 (our CPBIN4).
CPBRAS	CUM. SOLID CONC. PB-210 FROM RA-226 [mol m^{-3}]. The cumulative solid phase concentration of Pb-210 resulting from ingrowth from Ra-226 to TIME=t. Time dependent parameter used in the TSOURC modules and calculated from equation (3.11.7) of SENES Vol. 3. NOTE: The initial condition is CPBRAS=0 at TIME=0 (inspection of the UTAP2 code).
CPBRL2	CONC. PB-210 FROM INGROWTH IN ΔT, UNSAT. [mol m^{-3}]. The concentration of Pb-210 at the bottom of the unsaturated zone resulting from ingrowth from dissolved Ra-226 during the time step Δt. Intermediate time dependent variable used in the TSOURC modules and calculated using equation (3.11.3) of SENES Vol. 3. NOTE: The value for the radium concentration used here $[Ra_L]_{\lambda_w}$ is the value at TIME=t (SENES letter, 1986-12-02).
CPBRL3	CONC. PB-210 FROM INGROWTH IN ΔT, MIXING [mol m^{-3}]. The concentration of Pb-210 at the bottom of the mixing layer of the saturated zone resulting from ingrowth from dissolved Ra-226 during the time step Δt. Intermediate time dependent variable used in the TSOURC modules and calculated using equations (3.11.9) and (3.11.10) of SENES Vol. 3.
CPBRL4	CONC. PB-210 FROM INGROWTH IN ΔT, BOTTOM [mol m^{-3}]. The concentration of Pb-210 in the bottom layer of the saturated zone resulting from ingrowth from dissolved Ra-226 during the time step Δt. Intermediate time dependent variable used in the TSOURC modules and calculated using equations (3.11.11) and (3.11.12) of SENES Vol. 3.
CPBTI	INIT. CONC. PB-210 ASSOC. WITH HOST TAILINGS [mol m^{-3}]. Initial concentration of Pb-210 associated with host tailings material (not dissolved in the milling process and hence not associated with $PbSO_4$ in the tailings). This portion of the Pb-210 is assumed not to be leachable. Used in the TSOURC modules and calculated from equation (3.7.49) of SENES Vol. 3.
CRADI	INIT. SOLID PHASE CONC. RA-226 IN TAILINGS [mol m^{-3}]. The initial soild phase concentration of Ra-226 in the tailings. Used in the TSOURC modules and calculated from equation (3.7.35) of SENES Vol. 3.
CRADIN	NOTE: SENES uses CRADIN to refer to the radium inputs either to layer 3 (our CRAIN3) or to layer 4 (our CRAIN4). These are distinguishable as $[Ra]_{in}$ and $[Ra]_{in,1}$ (both defined as CRADIN) in SENES Vol. 3 Table A.3.
CRADTI	INIT. CONC. Ra-226 ASSOC. WITH HOST TAILINGS [mol m^{-3}]. Initial concentration of Ra-226 associated with host tailings material (not dissolved in the milling process and hence not associated with $BaSO_4$ in the tailings). This portion of the Ra-226 is assumed not to be leachable. Used in the TSOURC modules and calculated from equation (3.7.37) of SENES Vol. 3.
CRAIN3	CONC. RA MIXING ZONE INPUTS [mol m^{-3}]. The concentration of radium resulting from the various inputs to the mixing layer of the saturated zone. Time dependent intermediate parameter used in the

	TSOURC modules, and calculated using equations (3.10.32), (3.10.33) and (3.10.34) of SENES Vol. 3. The initial condition is specified by use of equation (3.10.33) for the time interval between TIME=-Δt and TIME=0. Equation (3.7.43) is not used for layer 3 (SENES letter, 1987-01-27). NOTE: SENES uses CRADIN to refer to either the inputs to layer 3 (our CRAIN3) or to layer 4 (our CRAIN4).
CRAIN4	CONC. RA BOTTOM ZONE INPUTS [mol m^{-3}]. The concentration of radium resulting from the various inputs to the bottom layer of the saturated zone. Time dependent intermediate parameter used in the TSOURC modules, and calculated using equations (3.10.38) and (3.10.39) of SENES Vol. 3. The initial condition is specified by use of equation (3.10.39) for the time interval between TIME=-Δt and TIME=0. Equation (3.7.43) is not used for layer 4 (SENES letter, 1987-01-27). NOTE: SENES uses CRADIN to refer to either the inputs to layer 3 (our CRAIN3) or to layer 4 (our CRAIN4).
CRATHS	CUM. SOLID CONC. RA-226 FROM TH-230 [mol m^{-3}]. The cumulative solid phase concentration of Ra-226 resulting from ingrowth from Th-230 to TIME=t. Time dependent parameter used in the TSOURC modules and calculated from equation (3.10.23) of SENES Vol. 3. NOTE: CRATHS=0.0 at TIME=-Δt and TIME=0 are the initial conditions (SENES letter, 1987-01-27 and inspection of the UTAP2 code).
CRATL2	CONC. RA-226 FROM INGROWTH IN ΔT, UNSAT. [mol m^{-3}]. The concentration of Ra-226 at the bottom of the unsaturated zone resulting from ingrowth from Th-230 during the time step Δt. Intermediate time dependent variable used in the TSOURC modules and calculated using equation (3.10.20) of SENES Vol. 3. NOTE: The thorium concentration required in this calculation is for TIME=t. (SENES 1986-12-02)
CRATL3	CONC. RA-226 FROM INGROWTH IN ΔT, MIXING [mol m^{-3}]. The concentration of Ra-226 resulting from ingrowth from Th-230 in the mixing layer of the saturated zone during the time step Δt. Intermediate time dependent variable used in the TSOURC modules and calculated using equations (3.10.26) and (3.10.27) of SENES Vol. 3. NOTE: The thorium concentration in this calculation is for TIME=t (SENES letter, 1986-12-02).
CRATL4	CONC. RA-226 FROM INGROWTH IN ΔT, BOTTOM [mol m^{-3}]. The concentration of Ra-226 resulting from ingrowth from Th-230 in the bottom layer of the saturated zone during the time step Δt. Intermediate time dependent variable used in the TSOURC modules and calculated using equations (3.10.28) and (3.10.29) of SENES Vol. 3.
CRO	RUNOFF REDUCTION FACTOR [-]. Runoff reduction factor used in the bedload transport capacity equation. Intermediate time dependent parameter used in the EROS module and calculated from equation (3.14.12) of SENES Vol. 3.
CSL	SOIL PERM. CLASS [-]. Soil permiability class. Input parameter used in the EROS module, and sampled from: Constant (5.0) (SENES letters, 1986-12-02, 1987-01-13).
CSOIL	CONTROL PRACTICE FACTOR [-]. Erosion control factor, treated here as exclusively a function of the amount of vegetation cover of the tailings. Intermediate parameter used in the EROS module and calculated from equation (3.14.6) of SENES Vol. 3 if FVEG>0, or assigned a value of 1.0 if FVEG=0. NOTE: See DDD 1.6.1.7 for additinal comments.

CT230I	INIT. SOLID PHASE CONC. OF TH-230 [mol m^{-3}]. Initial solid phase concentration of Th-230 in the tailings. Intermediate variable calculated from equation (3.7.14) of SENES Vol. 3:
CT232I	INIT. SOLID PHASE CONC. OF TH-232 [mol m^{-3}]. Initial solid phase concentration of Th-232 in the tailings. Intermediate variable calculated from equation (3.7.15) of SENES Vol. 3:
CTSOIL	TRANSPORT. REDN. FACTOR [-]. The transportability reduction factor used in the bedload transport capacity equation (given as a function of velocity with respect to bare soil for several slopes). Intermediate time dependent parameter used in the EROS module and calculated from equations 3.14.14 of SENES Vol. 3. NOTE: The equations were corrected in letters from SENES (1987-01-13 and 1987-01-27).
CURRNT	CURRENT VELOCITY [m a^{-1}]. Current velocity in the lakes of the watershed. Input parameter used in the WATEX module and sampled from: Uniform (3.15×10^4, 3.15×10^5)
CVEG(nuc,v,loc)	CONC. OF RADIONUCLIDE IN VEGETATION [Bq g^{-1}(wet weight)]. Average annual concentration of a radionuclide (nuc = nat-U, tot-Th, Ra-226, Pb-210) in vegetation of type (v) (types v=1,2,3,4,5 are above-ground and below-ground vegetables, summer forage, browse and lichen, respectively). The values are calculated at receptor locations - the specific sector and ring locations (1-80) for vegetables, the total study area for browse and lichens, the watershed area for summer forage. Values are due to foliar retention of the radionuclide deposited from dust in the air and to root uptake. Values are calculated as a function of time. Variable calculated in the VEGCON module and used as the variables AVEGC (v=1), BVEGC (v=2), SUFOC (v=3), BRWSC (v=4) and LICHC (v=5), in the VEGEAT or in the DOSE modules. The generic parameter CVEG(nuc,v,loc) has been used in the DDD's in the interests of clarity. Calculated using equation (8.1) of SENES Vol. 3.
D50	MEDIAN PARTICLE SIZE [mm]. The particle diameter size exceeeded by only 50% of the tailings particles. Intermediate parameter used in the EROS module and calculated using equation (3.14.10) of SENES Vol. 3.
DBAR	THICKNESS BASO4 DEPLETED LAYER [m]. The thickness of the barium sulphate depleted layer of the tailings. Intermediate variable used in the TSOURC modules and calculated using an equation below equation (3.10.6) of SENES Vol. 3. DBAR(TIME=t) = DBAR(TIME=(t-Δt)) +DHBAR The layer has been assumed by SENES to be 0.0 [m] thick at t=-Δt and 0.01 [m] thick at t=0 (see DBARZ below) (SENES Vol. 3, pg 3-81).
DBARZ	THICKNESS BASO4 DEPLETED LAYER AT TIME=0 [m]. The thickness of the barium sulphate depleted layer of the tailings at TIME=0. DBAR has been assumed by SENES to be 0.0 [m] thick at t=-Δt and has thickness DBARZ sampled from: Constant (0.01) at t=0 (SENES Vol. 3, pg 3-81).
DBOT	THICKNESS LAYER 4 [m]. The thickness of the bottom layer of the tailings (layer 4, below the mixing zone). Parameter used in the TSOURC modules and calculated (assuming a total tailings thickness of 10 [m]) from an equation given below equation (3.8.5) of SENES Vol. 3. DBOT = 10. - (DUNSAT + DMIX)

NOTE: Incorrectly given after equation (3.7.10) (SENES letter, 1986-12-02)

DCFGA(nuc) DCF FOR INGESTION OF NUC. (AIR) [μSv Bq^{-1}]. Whole body dose conversion factor for the ingestion of the radionuclide, nuc (nuc= nat-U, tot-Th, Ra-226, Pb-210), (air pathway). The values for nuc=nat-U, Ra-226, and Pb-210 are input parameters used in the DOSE module and sampled from:

Constant (6.7×10^{-2}) for nuc = nat-U
Constant (3.1×10^{-1}) Ra-226
Constant (1.4) Pb-210

and the value for total thorium is calculated using:

$$\text{DCFGA(tot-Th)} = (1.5 \times 10^{-1}) + \text{X232SA} \times (6.9 \times 10^{-1})$$

as given on page 13-5 of SENES Vol. 3. DCFGA(tot-Th) is time dependent.

NOTE: The term "natural thorium" is used in SENES Chapter 13 to refer to Th-232 plus Th-228 from the same decay chain.

DCFGW(nuc) DFC FOR INGESTION OF NUC. (WATER) [μSv Bq^{-1}]. Whole body dose conversion factor for the ingestion of the radionuclide, nuc (nuc= nat-U, tot-Th, Ra-226, Pb-210), (water pathway). The values for nuc=nat-U, Ra-226, and Pb-210 are input parameters used in the DOSE module and sampled from:

Constant (6.7×10^{-2}) for nuc = nat-U
Constant (3.1×10^{-1}) Ra-226
Constant (1.4) Pb-210

and the value for total thorium is calculated using:

$$\text{DCFGA(tot-Th)} = (1.5 \times 10^{-1}) + \text{X232LA} \times (6.9 \times 10^{-1})$$

as given on page 13-5 of SENES Vol. 3.

NOTE: The term "natural thorium" is used in SENES Chapter 13 to refer to Th-232 plus Th-228 from the same decay chain.

DCFHA(nuc) DCF FOR INHALATION OF NUC. [μSv Bq^{-1}]. Whole body dose conversion factor for the inhalation of the radionuclide, nuc (nuc= nat-U, tot-Th, Ra-226, Pb-210). The values for nuc=nat-U, Ra-226, and Pb-210 are input parameters used in the DOSE module and sampled from:

Constant (3.4×10^{1}) for nuc = nat-U
Constant (2.1) Ra-226
Constant (3.4) Pb-210

and the value for total thorium is calculated using:

$$\text{DCFGA(tot-Th)} = (7.0 \times 10^{1}) + \text{X232SA} \times (3.2 \times 10^{2})$$

as given on page 13-5 of SENES Vol. 3. DCFHA(tot-Th) is time dependent.

NOTE: The term "natural thorium" is used in SENES Chapter 13 to refer to Th-232 plus Th-228 from the same decay chain.

DCGWAT(nuc) DISTRIBUTION COEFFICIENT FOR RADIONUCLIDE [m^{3} kg^{-1}]. The ratio of the concentration of the radionuclide (nuc = nat-U, tot-Th, Ra-226, Pb-210) adsorbed on a unit mass of solid material, to the concentration of radionuclide in a unit volume of solution (e.g., groundwater). Input parameter in GWATER and sampled from:

LOG NORMAL (0.02, 2.5, 0.005, 0.5) uranium
(0.5, 2.15, 0.05, 5.) thorium
(0.67, 1.73, 0.13, 3.5) lead
(0.07, 1.9, 0.01, 0.5) radium

NOTE: These differ from the distributions provided for SOILKD in the SOIL module because the latter represent values for all conditions while DCGWAT is for pH 3-5.

DDD	DATA DEPENDENCY DIAGRAM. Part of the specifications, showing how parameters are combined to produce a calculated variable. More details are provided in Appendix B.
DELT	SO4 COMPLEX CORR. FACTOR [-]. Factor (dependent on pH) to obtain the free sulphate concentration from the total sulphate concentration. Parameter used in the TSOURC modules and calculated from equation (3.3.38) of SENES Vol. 3. NOTE: See DDDs 1.1.2.8 and 1.1.2.9 for additional comments affecting the calculation of DELT.
DELTAG	GYP. DISS. IN MIXING ZONE IN TIME INT. [mol m^{-3}] The amount of gypsum (per unit volume) dissolved in the mixing zone between TIME=(t-Δt) and TIME =t. Intermediate variable used in the TSOURC modules and calculated using equation (3.4.9) of SENES Vol. 3.
DELTAH	INCREMENTAL CHANGE IN DGYP [m]. Incremental change in the depth of the upper (gypsum-depleted) layer of the unsaturated zone from time = TIME to time = TIME+DT. Intermediate variable calculated in the TSOURC modules. Calculated from equations (3.3.26) and (3.3.65) of SENES Vol 3. The equation used depends on whether limestone is present. $\text{DELTAH} = \text{DGYP(at TIME} = t) - \text{DGYP(at TIME} = (t-\Delta t))$ (for DGYP < DUNSAT) $\text{DELTAH} = 0$ (for DGYP = DUNSAT) DELTAH is an intrinsically non-negative variable, with a value of zero at TIME= -Δt and when DGYP = DUNSAT, and with positive values in between.
DEPVEL	DEPOSITION VELOCITY [m s^{-1}]. Deposition velocity for radionuclides in dust particulates. Input parameter used in the SOIL and VEGCON modules, and sampled from: Uniform (0.003, 0.03)
DETIME(n)	RETENTION TIME IN LAKE n [a]. Retention time (or travel time) in a lake between node (n-1) and node n. Variable calculated in the LAKEPH module and used in the WATEX and LAKEPH modules. Calculated using an equation following equation (10.29) in SENES Vol. 3: $\text{DETIME}(n) = \text{LAKVOL}(n) / \text{FLOWQ}(n)$
DF	DEPTH OF FLOW [ft]. Depth of flow for average erosion using a two-year period peak discharge flowing over the area. Intermediate time dependent parameter used in the EROS module, but not defined in SENES Vol. 3. The equation: $\text{DF}=(\text{STORM} \times \text{LENGT})/(2.633 \times 10^7 \times \text{VEL}$ was given in a letter from SENES (1987-01-13).
DFD	DATA FLOW DIAGRAM. Part of the specifications, showing the movement of data from one process bubble to another. More details are provided in Appendix B.
DFR(nuc)	RADIONUCLIDE DECAY FACTOR [-]. Factor to allow for the decay of radionuclide during the residence time in lake water or lake sediments (nuc=Ra-226, Pb-210). Intermediate parameter used in the WATEX module. Not noted specifically in Chapter 10 of SENES Vol. 3, but calculated from portions of the equations given on page 10-30.
DGYP	DEPTH OF UPPER UNSAT. ZONE [m]. Depth of the gypsum depleted (upper) portion of the unsaturated zone. Time dependent parameter calculated and used in the TSOURC modules, and calculated from equations (3.3.27) and (3.3.28) of SENES Vol. 3. NOTE: The initial condition is DGYP=0 (inspection of the UTAP2 code). NOTE: By definition, the maximum value of DGYP is DUNSAT.

DHBAR	INCR. BASO4 DEPLETED LAYER [m]. Increase in the thickness of the barium sulphate depleted layer over the time interval Δt. Time dependent intermediate variable used in the TSOURC modules and calculated using equation (3.10.6) of SENES Vol. 3.
DHLEAD	INCR. PBSO4 DEPLETED LAYER [m]. Increase in the thickness of the lead sulphate depleted layer over the time interval Δt. Intermediate time dependent variable used in the TSOURC modules and calculated using equation (3.11.4) of SENES Vol. 3.
DIFFC	SEDIMENT DIFFUSIVITY COEFFICIENT $[m^2\ a^{-1}]$. Diffusivity coefficient for lake sediment. Input parameter used in WATEX and sampled from: Constant (0.02)
DIFLEN	RECIPROCAL OF RN DIFFUSION PATH LENGTH $[m^{-1}]$. Reciprocal of the Rn-222 diffusion path length. Intermediate variable calculated in the RADON module. Calculated using an equation near equation (4.1) in SENES Vol. 3: $DIFLEN = [\ RNLAM \times POROS\ /\ EBKDFC\ ]^{0.5}$
DLEAD	THICKNESS PBSO4 DEPLETED LAYER [m]. The thickness of the lead sulphate depleted layer of the tailings. Intermediate variable used in the TSOURC modules and calculated using equation (3.11.5) of SENES Vol. 3. $DLEAD(TIME=t) = DLEAD(TIME=(t-\Delta t)) + DHLEAD$ The layer has been assumed by SENES to be 0.0 [m] thick at $t=-\Delta t$ and 0.01 [m] thick at t=0 (see DLEADZ below) (SENES Vol. 3, pg 3-93).
DLEADZ	THICKNESS PBSO4 DEPLETED LAYER AT TIME=0 [m]. The thickness of the lead sulphate depleted layer of the tailings at TIME=0. DLEAD has been assumed by SENES to be 0.0 [m] thick at $t=-\Delta t$ and has thickness DLEADZ sampled from: Constant (0.01) at t=0 (SENES Vol. 3, pg 3-93).
DM	MEAN METRIC SILT DIAMETER [mm]. The mean diameter of silt particles from the tailings expressed in millimetres. Input parameter used in the EROS module, not given in SENES Vol. 3, but noted in a letter (1987-01-13) from SENES. In the same letter it was indicated the parameter should be sampled from: Constant (0.01)
DMID	MEAN SILT DIAMETER [ft]. The mean diameter of silt particles from the tailings. Intermediate parameter used in the EROS module, not defined in SENES Vol. 3, but given in a letter (1987-01-13) from SENES. Calculated from: DMID = DM / (308.4)
DMIX	THICKNESS OF MIXING ZONE [m]. Thickness of the mixing zone, which is part of the saturated zone underlying the unsaturated zone. It is assumed that the source of contaminated surface waters derives from releases from the mixing zone. Input parameter used in the TSOURC modules and sampled from: Uniform (1.0, 2.0)
DOSE	MODULE. All processes required to calculate ootal internal dose to a critical (and average) receptor, given concentrations of contaminants (U, Th, Ra, Pb and Rn) in air, soil and water at the receptors location (see DFD 4.0 to 4.4 inclusive). The major outputs from DOSE are DOSEIA and DOSEIC. Other important outputs are VEGD, WATD, FISHD, etc.
DOSEGS(loc)	TOTAL EXTERNAL DOSE RATE FROM GROUNDSHINE $[Sv\ a^{-1}]$. Total groundshine dose rate at the receptor locations (loc=1,80) summed

over all decay chains (U-238, Th-tot, Ra-226 (total), Pb-210). Major output, calculated in the GSHINE module from the sum of terms of the type given on the left-hand side of the equation on page 7-10 of SENES Vol. 3.

DOSEIA TOTAL INTERNAL DOSE (AR) [μSv a^{-1}]. Total internal dose to an average receptor due to ingestion of contaminated vegetables, caribou, moose, fish and drinking water, and due to the inhalation of contaminants in dust and radon and its daughters. Final time dependent output of the DOSE module; not defined by SENES, but given by a sum of DOSET(nuc) (nuc = U-nat, Th-tot, Ra-226, Pb-210, Rn)

DOSEIC TOTAL INTERNAL DOSE (CR) [μSv a^{-1}]. Total internal dose to a critical receptor due to ingestion of contaminated vegetables, caribou, moose, fish and drinking water, and due to the inhalation of contaminants in dust and radon and its daughters. Final time dependent output of the DOSE module; not defined by SENES, but given by a sum of DOSET(nuc) (nuc = U-nat, Th-tot, Ra-226, Pb-210, Rn)

DRYRHO DRY SOIL DENSITY [g m^{-3}]. The dry density of the soil. Used in the VEGCON module, and calculated as:

RHOS(2) x 1000.

NOTE: Confirmed in SENES letter (1986-10-15).

DSOIL(sla) DEPTH OF SOIL LAYER [m]. Depth of the layer of soil, sla (sla=1,NLAYER). Input parameter used in the SOIL and GSHINE modules, and sampled from:

Constant(0.05) sla=1
(0.15) sla=2

The 1st layer is the surface layer, the 2nd layer is the uppermost subsurface layer.

DT≡Δt TIME STEP-SIZE [a]. Time step-size used within various equations, such as the finite difference equation for WATCCA. Input parameter used in the TSOURC, SOIL and LAKEPH modules. Not specified, but assigned values of 1-10 [a] in Table 2.1 of SENES Vol. 3.

DUNSAT DEPTH OF UNSAT. ZONE [m]. Depth of the unsaturated zone, including the upper ($BaSO_4$ and gypsum depleted) and lower ($BaSO_4$ and gypsum enriched) layers. Input parameter used in the TSOURC and RADON modules and sampled from:

Uniform (0.75, 1.25) in TSOURC

The distribution Uniform (0.5, 1.0) in given in RADON. A letter dated 1986-11-04 indicates the value of DUNSAT is assigned in the TSOURC module (Uniform (0.75, 1.25)), and this value is directly transferred to RADON. Therefore, the value assigned in TSOURC is almost certainly correct, and that in Table 4.1 of SENES Vol. 3 incorrect.

DUREXP(v) DURATION OF EXPOSURE OF VEGETATION [s]. Duration of exposure of vegetation types v=1,2,3,4,5 (above-ground and below-ground vegetables, summer forage, browse and lichen). Input parameter used in the VEGCON module and sampled from:

Triangular (2.6×10^6, 5.2×10^6, 7.8×10^6) (v=1,2)
Uniform (1.3×10^6, 3.9×10^6) (v=3,4)
Constant ($1. \times 10^{10}$) (v=5)

DUSDIA INTERNAL DOSE (AR) FROM DUST [μSv a^{-1}]. Internal dose to an average receptor due to inhalation of contaminants in dust. Major time dependent output from the DOSE module. No equation given in SENES, but calculated from the sum of all nuclide doses to the receptor from dust inhalation.

DUSDIC INTERNAL DOSE (CR) FROM DUST [$\mu Sv\ a^{-1}$]. Internal dose to a critical receptor due to inhalation of contaminants in dust. Major time dependent output from the DOSE module. No equation given in SENES, but calculated from the sum of all nuclide doses to the receptor from dust inhalation.

DUST MODULE: EMISSION RATE OF RADIONUCLIDE IN DUST FROM TAILINGS SURFACE. All processes required to calculate the emission rate of radionuclides associated with dust at the tailings surface (see DFD 2.0 and DDD 2.1). The major output values from DUST is EMRATE(nuc), nuc = nat-U, tot-Th, Ra-226, Pb-210.

DV DARCY VELOCITY [$m\ a^{-1}$]. The Darcy velocity of the groundwater through the aquifer. Intermediate variable used in the GWATER module and calculated using equation 9.2 of SENES Vol. 3.

EBKDFC EFFECTIVE BULK DIFFUSION COEFFICIENT [$m^2\ s^{-1}$]. Effective bulk diffusion coefficient of Rn-222 in the unsaturated zone of the tailings. Intermediate variable calculated in the RADON module. Calculated using equation 4.3 in SENES Vol. 3:

$$EBKDFC = 0.106\text{x}10^{-4} \text{ x } POROS \text{ x } EXP\ [-0.261 \text{ x } MPCH20]$$

NOTE: the constants in the above equation are not defined nor described further in the SENES report.

EFR EQUIL. FACTOR FOR RN [-]. The fraction of ingrowth of radon daughter isotopes at the receptor location. Input parameter used in the DOSE module and sampled from:

Triangular (0.2, 0.5, 0.8)

EMANAT EMANATION COEFFICIENT [-]. Radon emanation coefficient from the upper and lower layers of the unsaturated zone. Input parameter used in the RADON module and sampled from:

Triangular (0.02, 0.2, 0.9)

EMFRAC EMANATION COEFFICIENT SOIL[-]. Radon emanation coefficient from the soil. Input parameter used in the GSHINE module and sampled from:

Constant = (0.2)

EMRATE(nuc) ANN. AVG. EMISSION RATE OF RADIONUCLIDE IN DUST FROM TAILINGS [$Bq\ s^{-1}$]. Annual average emission rate of radionuclide (nuc= nat-U, tot-Th, Ra-226, Pb-210) in dust from the tailings surface, as a function of time. Time dependent variable calculated in the DUST module. Calculated using an equation on page 4-7 of SENES Vol. 3.

EMRATE(RN) ANN. AVG. EMISSION RATE OF RN GAS FROM TAILINGS [$Bq\ s^{-1}$]. Annual average emission rate of Rn-222 gas from the tailings unsaturated zone (upper and lower layers) as a function of time. Time dependent variable calculated in the RADON module. Calculated using equation (4.6) of SENES Vol. 3:

EMRATE(RN) = RNFXAV x ATAIL

ENERGY(nuc,band) AVG. ENERGY FOR RADIONUCLIDE CHAIN IN ENERGY BAND [MeV]. The average decay energy in a particular energy band for a selected radionuclide chain (nuc), (including daughter products in the decay chain). Intermediate parameter used in the GSHINE module sampled from:

Constants (SENES letter, 1986-10-15, 1986-11-04, 1987-02-03):

	ENERGY LEVELS				
DECAY CHAIN	1	2	3	4	5
U238 - U234	7.90E-02	0.0	0.0	9.10E-01	0.0
Th232-Pb208	5.96E-02	2.63E-01	5.67E-01	9.00E-01	2.57E-00

Pb210	4.7 E-02	0.0	0.0	0.0	0.0
Ra226(only)	1.86E-01	0.0	0.0	0.0	0.0
Rn222-Pb206	4.7 E-02	3.31E-01	6.09E-01	1.12E-00	1.76E-00

The total radium chain is the sum of the Ra226 and Rn222-Pb206 chains. Because of emission of radon from soil, the energy in each band for groundshine dose calculations must be devived from the values for the two chains using equation (7.9) of SENES Vol. 3. In the DDD's the Ra226 chain is referred to as (Ra°, radium only), and the value from the calculation for the total radium chain is noted as (Ra, radium).

EQUIL	SQ. ROOT OF EQBM. CONST. GYPSUM[mol m^{-3}]. EQUIL is an intermediate parameter, equal to the square root of the solubility product for gypsum, divided by the activity coefficient. Intermediate variable calculated in and used throughout the TSOURC modules. EQUIL is calculated using an expression near equation (3.3.22) in SENES Vol. 3: $EQUIL = (KSUBSO)^{1/2} / FACTCO$
EQUILB	SQ. ROOT OF EQBM. CONST. BASO4[mol m^{-3}]. EQUILB is an intermediate variable, equal to the square root of the solubility product for barium sulphate, divided by the activity coefficient. Intermediate variable calculated in and used throughout the TSOURC modules. EQUILB is calculated using an expression near equation (3.10.6) in SENES Vol. 3: $EQUILB = (KSBAR)^{1/2} / FACTCO$
EQUILP	SQ. ROOT OF EQBM. CONST. PBSO4[mol m^{-3}]. EQUILP is an intermediate variable, equal to the square root of the solubility product for lead sulphate, divided by the activity coefficient. Intermediate variable calculated in and used throughout the TSOURC modules. EQUILB is calculated using an expression near equation (3.11.4) in SENES Vol. 3: $EQUILP = (KSLEAD)^{1/2} / FACTCO$
EROS	MODULE. All processes required to calculate the mass loss of tailings to the watershed, through erosion (see DFD 1.6). The major outputs from EROS are EROTOT and AEXPT.
EROTOT	EROSION MASS LOSS FROM TAILINGS [kg]. The total sediment mass leaving the tailings pile in the time interval Δt. Major time dependent output of the EROS module, used in the WATEX module, and calculated from equation (3.14.21) of SENES Vol. 3. NOTE: See DDD 1.6.3.10 for a correction to this equation.
ESOIL	SEDIMENT DETACHED IN SEGMENT "eseg" [lb ft^{-1} a^{-1}]. The quantity of material eroded annually from the tailings pile in segment "eseg", as calculated from the Universal Soil Loss Equation. Intermediate time dependent parameter used in the EROS module and calculated from equation (3.14.2) of SENES Vol. 3 as modified in a letter from SENES (1987-01-27).
FACTCO	ACTIVITY COEFF. FOR DIVALENT IONS [-]. Activity coefficient for divalent ions, for use in the unsaturated zone where the ionic strength is expected to be high. Input parameter used in the TSOURC modules and sampled from: Triangular (0.3, 0.4, 0.5)
FAIAM	MOOSE AQUATIC FRACTION [-]. Fraction of annual feed intake that is local aquatic macrophytes. Parameter used in the DOSE module and calculated from an equation below equation (12.4) on page 12-9 of SENES Vol. 3.

FAIBM	MOOSE BROWSE FRACTION [-]. Fraction of annual intake that is local browse vegetation. Input parameter used in the DOSE module and sampled from: Triangular (0.8, 0.9, 0.95)
FAILC	FRAC. OF INTAKE - LICHEN [-]. Fraction of annual intake that is local lichen. Input parameter used in the DOSE module and sampled from: Triangular (0.05, 0.2, 0.5)
FAISFC	FRAC. OF INTAKE - FORAGE [-]. Fraction of annual intake that is local summer forage. Input parameter used in the DOSE module and sampled from: Triangular (0.05, 0.2, 0.5)
FDEPED(v)	FRACTION ON EDIBLE PORTION [-]. Fraction of contaminants deposited on vegetation type v that is retained on edible portions. Vegetation types v=1,2,3,4,5 are above-ground and below-ground vegetables, summer forage, browse and lichen. Input parameters used in the VEGCON module and sampled from: Uniform (0.8, 1.0) (v=1,3,4,5) Uniform (0.05, 0.15) (v=2) NOTE: These values are not entirely consistent with those in table 8.2 of the SENES report.
FDEPSF(v)	FRACTION OF DEPOSITION RETAINED [-]. Fraction of total deposition of contaminants that is retained on the surface of vegetation type v. Vegetation types v=1,2,3,4,5 are above-ground and below-ground vegetables,summer forage, browse and lichen. Input parameters used in the VEGCON module and sampled from: Uniform (0.1, 0.3) (v=1,2) Normal (0.47, 0.3, 0.01, 1.0) (v=3,4) Uniform (0.8, 1.0) (v=5)
FFLOC	FRAC. OF FISH LOCAL [-]. Fraction of annual fish intake that is local fish. Receptor specific input parameter used in the DOSE module and sampled from: Constant (1.0) - critical receptor Uniform (0.0,0.1) - average receptor
FIRC	FEED RATE FOR CARIBOU [g(wet) d^{-1}]. The average daily feed intake rate for caribou. Input parameter used in the DOSE module and sampled from: Triangular (5.0 X 10^3,7.0 X 10^3,9.0 X 10^3).
FIRM	FEED RATE FOR MOOSE [g(wet) d^{-1}]. The average daily feed intake rate for moose. Input parameter used in the DOSE module and sampled from: Constant (27.0 X 10^3).
FISH	MODULE. All processes required to calculate the concentration of radionuclide (U, Th, Ra, Pb) in edible fish flesh (see DFD 4.1.5). This is a very simple module, and the corresponding specification figures include the calculation of the major output variable FISHD.
FISHA(n)	FISH AVAILABILITY [-]. The fraction of fish available at the pH of the watershed at node "n" compared to the normal population of fish expected to be available if pH > 6. Intermediate time dependent parameter used in the DOSE module and calculated using equation (11.1) of SENES Vol. 3.
FISHC(nuc,n)	FISH CONC. [Bq g^{-1}(wet)]. Concentration of the radionuclide "nuc" in game fish flesh (nuc = U-nat, Th-tot, Ra-226, Pb-210) at watershed node "n". Time dependent parameter used in the DOSE module and calculated from equation (11.2) of SENES Vol. 3.

NOTE: There is an inconsistency in the units used for FISHC in SENES Table 11.5 and below SENES equation 11.2. The units in Table 11.5 are correct (SENES letter, 1987-01-27).

FISHD(nuc,n) INGEST. OF FISH DOSE [μSv a^{-1}]. Average annual whole body dose of radionuclide "nuc" (nuc = nat-U, tot-Th, Ra-226, Pb-210) from ingestion of fish for a specific location (watershed node) and receptor type. Intermediate time dependent parameter used in the DOSE module and calculated using equation (13.5) of SENES Vol. 3.

FISHIN ANN. INTAKE OF FISH [g a^{-1}]. Average annual intake of fish. Receptor specific input parameter used in the DOSE module and sampled from:

Constant (8 X 10^3)

The same value was used for critical and average receptors.

FLEAD FRACT. PB SOLUBLE [-]. Fraction of the ^{210}Pb assumed to be soluble. Input parameter used in the TSOURC modules and sampled from:

Uniform (0.92, 0.98)

FLOWQ(n) FLOW AT NODE n [m^3 a^{-1}]. Annual volume of surface water flow at node n. Intermediate variable calculated in the LAKEPH module. Calculated from equation (10.1) of SENES Vol. 3.

NOTE: See DDDs 3.2.5 and 3.2.5A for additional comments pertaining to FLOWQ(1).

FLXSL(nuc,band,sla,loc) FLUX FROM A SOIL LAYER [γ-rays m^{-2} s^{-1}]. The γ-flux in a particular energy band (band=1,NBAND) from a particular decay chain (U-238, nat-Th, Ra-226, Pb-210) for a particular soil layer (sla=1,NLAYER). Intermediate variable calculated in the GSHINE module for each receptor location (loc=1,80) using equation 7.3 of SENES Vol. 3.

FLXTOT(nuc,band,loc) TOTAL SOIL SURFACE FLUX [γ-rays m^{-2} s^{-1}]. The total γ-flux in a particular energy band (band=1,NBAND)at the soil surface from a specific decay chain (U, Th, Ra-226, Pb-210). Intermediate variable calulated in the GSHINE module using equation (7.12) of SENES Vol. 3.

FMTCC(nuc) CARIBOU XFR COEFF. [Bq g^{-1}(wet flesh) Bq^{-1} d]. The feed-to-caribou meat transfer coefficient for radionuclide (nuc). Input parameter used in the DOSE module and sampled from:

Triangular (1.1×10^{-7}, 3.4×10^{-7}, 1.0×10^{-6}) nuc = U-nat
(0.7×10^{-7}, 2.0×10^{-7}, 6.0×10^{-7}) nuc = Th-tot
(1.3×10^{-7}, 4.0×10^{-7}, 1.2×10^{-6}) nuc = Pb-210
(1.7×10^{-7}, 5.1×10^{-7}, 1.5×10^{-6}) nuc = Ra-226

FMTCM(nuc) MOOSE XFR COEFF. [Bq g^{-1}(wet flesh) Bq^{-1} d]. The feed-to-moose meat transfer coefficient for radionuclide (nuc). Input parameter used in the DOSE module and sampled from:

Triangular (1.1×10^{-7}, 3.4×10^{-7}, 1.0×10^{-6}) nuc = U-nat
(0.7×10^{-7}, 2.0×10^{-7}, 6.0×10^{-7}) nuc = Th-tot
(1.3×10^{-7}, 4.0×10^{-7}, 1.2×10^{-6}) nuc = Pb-210
(1.7×10^{-7}, 5.1×10^{-7}, 1.5×10^{-6}) nuc = Ra-226

FNG(nuc) GREEN'S FUNCTION [-]. The Green's function needed for the calculation of the time dependent radionuclide concentrations in groundwater (nuc nat-U, tot-Th, Ra-226, Pb-210). Intermediate time dependent variable used in the GWATER module and calculated from equation 9.12 of SENES Vol. 3.

NOTE: FNG=0 at t=0. At other times, its value is reset to zero if its calculated value is less than 1.0E-30 (inspection of the UTAP2 code).

FNPRCP	FRACT. NET PRECIP. [-]. Fraction of net precipitation that infiltrates the total depth of the tailings pile and enters zone 4 of the saturated zone. Input parameter used in the TSOURC and GWATER modules and sampled from: LOG NORMAL (0.15, 1.27, 0.07, 0.3) NOTE: Value is from Table A.3. The distribution in Table 3.4 is apparently incorrect (SENES letter 1986-10-15)
FPREC	ANNUAL DAYS WITH SIG. PRECIP. [d a^{-1}]. Annual number of days with more that 0.25 mm of precipitation, excluding winter months. Input parameter used in the DUST module and sampled from: Normal (123.0,18.0,84.0,156.0) NOTE: If FPREC is sampled annually the above distribution should be used. If the parameter is sampled only at the beginning of each trial, then the distribution must be adjusted for the time period of the simulation. (as noted by SENES in a letter dated 15-Oct-1986).
FRACGP	MASS FRAC. OF GYPSUM IN TAILINGS [-]. Mass fraction of gypsum in tailings. Input parameter used in the TSOURC modules and sampled from: Uniform (0.05, 0.06)
FRACTH	FRAC. OF TH(OH)4 CRYSTALLINE [-]. Fraction of the $Th(OH)_4$ which is crystalline. Input parameter used in the TSOURC modules and sampled from: Triangular (0.2, 0.3, 0.4)
FRACU	FRACT. U308 ASSOC. WITH PYRITE [-]. Fraction of the U_3O_8 in the tailings that is associated with pyrite. Input parameter used in the TSOURC modules and sampled from: Uniform (0.3, 0.9)
FRAD	FRACT. RA SOLUBLE [-]. Fraction of the ^{226}Ra which is assumed to be soluble. Input parameter used in the TSOURC modules and sampled from: Triangular (0.25, 0.60, 0.95)
FSHDIA	INTERNAL DOSE (AR) FROM FISH [μSv a^{-1}]. Internal dose to an average receptor due to ingestion of contaminated fish. Major time dependent output from the DOSE module. No equation given in SENES, but calculated from the sum of all nuclide doses to the receptor from fish ingestion.
FSHDIC	INTERNAL DOSE (CR) FROM FISH [μSv a^{-1}]. Internal dose to a critical receptor due to ingestion of contaminated fish. Major time dependent output from the DOSE module. No equation given in SENES, but calculated from the sum of all nuclide doses to the receptor from fish ingestion.
FT	WATERSHED ADJUSTMENT FACTOR [-]. An adjustment factor used to reflect the fact the watershed is only a fraction of the total area being modelled (i.e., the fraction of the total area considered that is in the watershed). Intermediate parameter used in the DOSE module and calculated in the way described at the bottom of page 12-6 of SENES Vol. 3 using: FT = SHEDDAR(8)/STDYAR.
FT230	FRACT. TH-230 SOLUBLE [-]. Fraction of the original ^{230}Th that is soluble in water. Input parameter used in the TSOURC modules and sampled from: Uniform (0.92, 0.98)
FT232	FRACT. TH-232 SOLUBLE [-]. Fraction of the original ^{232}Th that is soluble in water. Input parameter used in the TSOURC modules and

sampled from:
Uniform (0.60, 0.70)

FURAN MASS FRACT. U RECOVERED [-]. Mass fraction of uranium recovered in the mill. Input parameter used in the TSOURC models and sampled from:
Uniform (0.92, 0.98)

FVEG FRACT. TAILINGS VEG. [-]. Fraction of the surface area of the tailings pile that is vegetated. Intermediate time dependent parameter used in the EROS module. Calculated from equation 3.14.7 of SENES Vol. 3.
NOTE: FVEG has a maximum value of 0.9, and is defined as 0.0 if PH1 < 4 (text above and below equation 3.14.7).
NOTE: See DDD 1.6.1.7 for additional comments.

FWAT FRAC. OF NET PPTN. IN RUNOFF [-]. Fraction of the net precipitation that does not leach into the soil, and hence does not infiltrate the soil profile. Input parameter used in the SOIL module, and sampled from:
Triangular (0.02, 0.16, 0.48)

FWIND(dir,st,vel,yr) FRACTION OF WIND TYPE [-]. Fraction of the wind of direction dir (1->16), stability class st (1->6), velocity class vel (1->6) in sample year n. A single entry in the AES STAR files for wind data. Not used explicitly in SENES Vol. 3, but needed for the calculation of FWIND1, FWIND2, FWINDT and UWIND. The STAR files contain the values for twenty years. Input in the AIRDIS module and sampled or calculated from the STAR tables.
NOTE: SENES used values of FWIND in at least two ways. The first was to obtain a twenty year average value for each element. The second, for some runs with ten year time steps, was to sample from a set of twenty ten-year averages. The ten year averages were derived by cyclicly permuting the twenty year data (i.e., years 1-10, 2-11, ... 11-20, 12-20 & 1, 13-20 & 1-2, etc.). Presumably they may also have sampled from the array of single year data for one year time steps.
NOTE: The STAR data file is input in an unusual order, as noted in comment 132 of Appendix A.

FWIND1(d) FRACTION OF TIME WIND BLOWS TO RECEPTOR WITH HIGH WIND SPEEDS [-]. Fraction of the time the wind blows from the tailings source to the receptor (a 'critical' man or vegetation) (i.e., in a particular direction, with high wind speeds (velocities > 5.4 $m \cdot s^{-1}$). Calculated from STAR data using an equation supplied in a letter by SENES (1986-11-04):

$$FWIND1 = \sum_{s=1}^{6} \sum_{v=4}^{6} FWIND(d,s,v,n),$$

however it is not clear where (or if) FWIND1 is required. Note: inspection of the SENES code shows that FWIND1 is used as shown in DDD 2.3.5.

FWIND2(dir,st) FRACTION OF TIME WIND BLOWS TO RECEPTOR [-]. Fraction of the time the wind blows from the tailings source to the receptor (a man or vegetation) in a particular direction "dir" with a particular atmospheric stability "st". Used in the AIRDIS module and calculated from STAR data using the equation:

$$FWIND2(dir,st) = \sum_{vel=1}^{6} FWIND(dir,st,vel,n)$$

Described in a letter from SENES (1986-11-04)

FWINDT FRACTION OF TIME WITH HIGH WIND SPEEDS [-]. Fraction of the time that the wind speed over the tailings surface exceeds 5.4 m s^{-1} at the mean tailings height (HSRC). Input parameter used in the DUST module and calculated in the WIND subroutine. The details of the calculation do not appear in SENES Vol. 3. Calculated from STAR data using an equation suppled in a letter from SENES (1986-11-04):

$$\mathrm{FWINDT} = \sum_{dir=1}^{16} \sum_{st=1}^{6} \sum_{vel=4}^{6} \mathrm{FWIND}(dir,st,vel,n)$$

GDOS(nuc,band,loc) BAND GROUNDSHINE DOSE [Sv a^{-1}]. Groundshine dosefrom each energy band (band=1,NBAND) at a receptor (loc=1,80) from a particular radionuclide decay chain (nuc=U-238, Th, Ra-226(total), Pb-210). Intermediate variable calculated in the GSHINE module using the equation (7.13) of SENES Vol. 3.

GDOSN(nuc,loc) TOTAL GROUNDSHINE DOSE RATE FOR RADIONUCLIDE CHAIN[Sv a^{-1}]. Total groundshine dose at a receptor (loc=1,80) from a radionuclide decay chain (nuc=U-238, Th, Ra-226(total),Pb-210). Intermediate variable calculated in the GSHINE module using the equation on page 7-10 of SENES Vol. 3.

GSHINE MODULE. All processes required to calculate the total groundshine dose at a particular receptor location from all radionuclides decay chains and energy levels (see DFD 2.5). The major output is DOSEGS.

GWATC(nuc) GROUNDWATER RADIONUCLIDE DISCHARGE CONC.[Bq m^{-3}]. The radionuclide concentration at the discharge from the aquifer (nuc=nat-U, tot-Th, Ra-226, Pb-210). Major time dependent output variable calculated in the GWATER module using equation 9.15 and, for Pb-210 only, equations 9.8a and 9.8b of SENES Vol. 3.
NOTE: GWATC(nuc)=0 at t=0 (inspection of the UTAP2 code).

GWATER MODULE. All processes required to calculate the concentrations of the radionuclides at the discharge point of the aquifer (see DFD 3.1). The major output is GWATC.

GWATP(nuc) DISCHARGE CONCENTRATION NOT INCLUDING IN-GROWTH [Bq m^{-3}]. The radionuclide concentration at a particular time at the discharge from the aquifer (nuc= nat-U, tot-Th, Ra-226, Pb-210). Does not include in-growth of Pb-210 from Ra-226. Intermediate time dependent variable calculated in the GWATER module and calculated using equation 9.15 of SENES Vol. 3.

GYPI INIT. GYPSUM CONTENT IN TAILINGS [mol m^{-3}]. Initial gypsum content of tailings. This apparently refers to the bulk tailings. Intermediate variable calculated in and used throughout the TSOURC modules. Calculated from equation (3.2.2) in SENES Vol. 3:

$$\mathrm{GYPBLK} = \mathrm{RHOTAL} \times \mathrm{FRACGP} / 136$$

GYPMIX GYP. DISS. IN MIXING ZONE [mol m^{-3}] The total gypsum per unit volume dissolved in the mixing zone to any TIME = t. Intermediate variable used in the TSOURC modules and calculated using a slightly modified version of equation (3.4.10) of SENES Vol. 3.

HSRC HEIGHT OF SOURCE [m]. Mean height of the tailings source. Input parameter used in the AIRDIS module and sampled from:

Uniform (1.0, 3.0)

IGPB INGROWTH FACTOR FOR PB-210 [-]. The factor used to approximate the ingrowth of Pb-210 from Ra-226. Intermediate parameter used in the TSOURC module and the WATEX module. This parameter is not explicitly defined by SENES, but appears as parts of many equations such as (3.11.10) and (3.11.12).

IGRA	INGROWTH FACTOR FOR RA-226 [-]. The factor used to approximate the ingrowth of Ra-226 from Th-230. Intermediate parameter used in the TSOURC module and the WATEX module. This parameter is not explicitly defined by SENES, but appears as parts of many equations such as (3.10.23) and (3.10.27).
INHD(nuc,loc)	DUST DOSE [μSv a^{-1}]. Average annual whole body dose of radionuclide "nuc" (nuc = nat-U, tot-Th, Ra-226, Pb-210) from inhalation of dust for a specific location and receptor type. Intermediate time dependent parameter used in the DOSE module and calculated using equation (13.6) (incorrectly labelled equation (11.1) on page 13-15) of SENES Vol. 3.
INLIME	INVENT. CACO3 [mol m^{-3}]. The residual concentration of limestone or calcite (as $CaCO_3$) in the unsaturated layer at time t. Intermediate parameter used in the TSOURC modules. Not noted by SENES but derived from equation (3.3.70) of SENES Vol. 3 using: INLIME = LIMEIN - [Σ(CALIME x NPRCP x DT)]/DUNSAT INLIME is not explicitly defined by SENES, but is required to determine if $CaCO_3$ is still present in the unsaturated zone at any particular time.
INOCC	FRAC. OUTDOORS [-]. The fraction of time the receptor is outdoors when at a specific location. Input parameter used in the DOSE module and sampled from: Triangular (0.5, 0.75, 0.9) The same value was used for critical and average receptors.
K1(nuc,n)	RATE CONST. FOR REMOVAL OF RADIONUCLIDE [a^{-1}]. Rate constant for removal of radionuclide nuc (nuc= U, Th, Ra, Pb) from the lake water column of the lake between watershed nodes (n-1) and n. Intermediate parameter used in the WATEX module and calculated from equation 10.26 of SENES Vol. 3
K2(nuc,n)	RATE CONST. FOR RELEASE OF RADIONUCLIDE [a^{-1}]. Rate constant for release of radionuclide nuc (nuc= U, Th, Ra, Pb) from the exchangeable sediment back to lake water column of the lake between watershed nodes (n-1) and n. Intermediate parameter used in the WATEX module and calculated from equation 10.27 of SENES Vol. 3
K3(nuc,n)	RATE CONST. FOR RADIONUCLIDE BURIAL[a^{-1}]. Rate constant for loss of radionuclide nuc (nuc= U, Th, Ra, Pb) to deep lake sediment of the lake between watershed nodes (n-1) and n. Intermediate parameter used in the WATEX module and calculated from equation 10.27 of SENES Vol. 3
KDLEAD	PB SOLID-LIQUID DISTR. COEFFICIENT [m^3 g^{-1}]. Lead solid-liquid distribution coefficient in the mixing zone. Input parameter used in the TSOURC modules and sampled from: Triangular (20.x10^{-6}, 60.x10^{-6}, 100.x10^{-6})
KDPRIM	SLOPE TH KD [m^3 g^{-1}]. The slope in the linear function relating the thorium distribution coefficient to pH(n,t). Input parameter used in the WATEX module and sampled from: Log Normal (2.0 x 10^{-2}, 2.5, 2.0 x 10^{-3}, 0.30) NOTE: Unit check fails if this parameter has dimensions [-] as in Table 10.5 of SENES Vol. 3.
KDRAD	RA SOLID-LIQUID TRANSFER COEFFICIENT [m^3 g^{-1}]. Radium liquid-solid transfer coefficient (also known as distribution coefficient) in the mixing zone. Input parameter used in the TSOURC modules and sampled from: Triangular (5.x10^{-6}, 40.x10^{-6}, 75.x10^{-6})

KDUO2	U SOLID-LIQUID DISTR. COEFF. [m^3 g^{-1}]. Uranium solid-liquid distribution coefficient in the mixing zone. Input parameter used in the TSOURC modules and sampled from: LogNormal ($3.x10^{-5}$, 3.0, $1.1x10^{-6}$, $8.1x10^{-4}$)
KFBAR	BASO4 FORMATION CONSTANT [m^3 mol^{-1}]. Formation constant for the aqueous species, $BaSO_4$. Input parameter used in the TSOURC modules and sampled from: Constant (5.01×10^{-1})
KFLEAD	PBSO4(AQ) FORMATION CONSTANT [m^3 mol^{-1}]. Formation constant for the aqueous species, $PbSO_4$. Input parameter used in the TSOURC modules and sampled from: Constant (5.01×10^{-1})
KPRIME	RATIO OF KO_2 TO [O_2] [-]. Ratio of O_2 half-saturation constant to [O_2]. Input parameter used in the TSOURC modules and sampled from: Lognormal (5×10^{-2}, 1.7, 0.02, 0.25)
KRAD	RA SOLID/AQ DIST. COEFFICIENT [-]. Radium solid/liquid distribution coefficient in the unsaturated zone. Input parameter used in the TSOURC modules and sampled from: Uniform (0.50, 0.56)
KRATE	RATE CONST. OF OXD'N OF PYRITE [a^{-1}]. Rate constant for oxidation of pyrite. Intermediate variable calculated in the TSOURC modules. Calculated from equation (3.3.10) of SENES Vol. 3: KRATE = SFLUX / (2 x DUNSAT x PYRITI)
KS(nuc,n)	KS PARAMETER USED IN WATEX [Bq]. Intermediate parameters used in the calculation of WATRW and WATRS in the WATEX module. This time dependent parameter is defined by an equation below equations (10.32) and (10.33) in SENES Vol. 3. NOTE: See DDD 3.3.8.3 for corrections to these equations.
KSBAR	SOLUBILITY EQM. CONST. FOR BASO4 [mol^2 m^{-6}]. Equilibrium constant for the dissolution of barium sulphate (solubility product constant). Input parameter used in the TSOURC modules and sampled from: Constant (1.07×10^{-4})
KSLEAD	SOLUBILITY EQM. CONST. FOR PBSO4 [mol^2 m^{-6}]. Equilibrium constant for the dissolution of lead sulphate (solubility product constant). Input parameter used in the TSOURC modules and sampled from: Constant (1.2×10^{-2})
KSOIL	SOIL ERODIBILITY FACTOR [-]. The factor in the universal soil loss equation that relates erosion to soil type. Intermediate parameter used in the EROS module, and calculated from equation 3.14.4 of SENES Vol. 3. NOTE: The value for the parameter "c (=5)" was provided by SENES in a letter (1986-12-02).
KSUBSO	SOLUBILITY EQBM. CONST. FOR GYPSUM [mol^2 m^{-6}]. Equilibrium constant for the dissolution of gypsum (solubility product constant). Input parameter used in the TSOURC modules and sampled from: Constant (25.0)
KW(nuc,n)	KW PARAMETER USED IN WATEX [Bq]. Intermediate parameters used in the calculation of WATRW and WATRS in the WATEX module. This time dependent parameter is defined by an equation below equations (10.32) and (10.35) in SENES Vol. 3. NOTE: See DDD 3.3.8.2 for corrections to these equations.
LAKEPH	MODULE. All processes required to calculate the pH in a lake lying between nodes (n-1) and n, given concentrations of relevant ions from the tailings source (see DFD 3.2). The major output from LAKEPH is WATPH.

LAKVOL(n) VOLUME OF LAKE n [m^3]. Volume of the lake in the watershed between nodes (n-1) and n. Intermediate parameter used in the LAKEPH and WATEX modules and calculated in the LAKEPH module from an equation on page 10-27 of SENES Vol. 3:

LAKVOL(n) = LAREA(n) x SDEPTH(n)

LAM230 TH-230 DECAY CONSTANT [a^{-1}]. Radioactive decay constant for Th-230. Input parameter used in the TSOURC and WATEX modules and sampled from:

Constant (8.66×10^{-6}) (as defined in Tables A.3 and 10.5 of SENES Vol. 3).

LAMDA(nuc) NUCLIDE DECAY CONSTANT [a^{-1}]. Radioactive decay constant for radionuclide. Input parameter used in the SOIL module, also required in the GWATER module, and sampled from:

Constant (1.53×10^{-10}) nuc = U-238
(4.92×10^{-11}) Th-232
LAMPB Pb-210
LAMRAD Ra-226

NOTE: It is not clear why the different symbols were used for the decay constants in the different modules. Furthermore, as confirmed by a letter from SENES (1986-12-11), the values for U-238 and Th-232 are not really the necessary data for the calculations (for nat-U and tot-Th). The decay of uranium and thorium is just so slow that it makes no difference over the time frame considered here. GWATER lists values for $t_{1/2}$ that result in equivalent values for LAMDA (λ) except for differences caused by rounding errors in the last "significant" figure (SENES letter, 1986-10-15).

LAMPB PB-210 DECAY CONSTANT [a^{-1}]. Radioactive decay constant for Pb-210. Input parameter used in the TSOURC, SOIL and WATEX modules, and sampled from:

Constant (3.3×10^{-2})

NOTE: LAMDA(PB) in Table 6.2 is LAMPB.

LAMRAD RA-226 DECAY CONSTANT [a^{-1}]. Radioactive decay constant for Ra-226. Input parameter used in the TSOURC and WATEX modules, and sampled from:

Constant (4.33×10^{-4}) (as defined in Tables A.3 and 10.5 of SENES Vol. 3).

NOTE: LAMDA(RA) in Table 6.2 is LAMRAD.

LAREA(n) AREA OF LAKE n [m^2]. Area of the lake in the watershed between nodes (n-1) and n. Input parameter used in the WATEX and DOSE modules and sampled from:

CONSTANT (0.0) n=1,3,5,6,8 (rivers)
(5.0×10^5) n=2
(2.5×10^5) n=4
(4.0×10^6) n=7

LDC LONGITUDINAL DISPERSION COEFFICIENT [m^2 a^{-1}]. The longitudinal dispersion coefficient. Intermediate variable used in the GWATER module and calculated using equation 9.4 of SENES Vol. 3.

LENGT TOTAL LENGTH OF TAILINGS PILE [ft]. The total length of the slope of the tailings pile. Intermediate parameter used in the EROS module and calculated from:

LENGT = (ATAIL)$^{0.5}$ / CFFM

as described in a letter from SENES (1987-01-13).

LENGTH LENGTH OF A SLOPE SEGMENT [ft]. The length of each segment of the tailings pile such that there is a minimum number of equal-length segments each less than 400 ft. in length. Intermediate parameter used in the EROS module and calculated from:

LENGTH = LENGT / NLEN

according to the discussion on page 3-124 of SENES Vol. 3 and a letter from SENES (1987-01-13).

LENTOT(eseg) TOTAL LENGTH TO END SEGMENT "eseg" [ft]. The total length of the slope of the tailings pile from the top to the bottom of segment "eseg". Intermediate parameter used in the EROS module calculated in the method described by SENES in a letter (1987-01-13):

LENTOT(eseg) = LENGTH x eseg

calculated for all tailings pile segments from 1 to NLEN.

LICHC(nuc) CONC. OF RADIONUCLIDE IN LICHENS [Bq g^{-1}(wet weight)]. Average annual concentration of radionuclide (nuc) in lichens due to foliar retention of the radionuclide deposited from dust in the air and with root uptake assumed to be nil. Values are calculated as a function of time and location. Variable calculated in the VEGCON module and used in the DOSE module. Calculated using equation (8.1) of SENES Vol. 3.

NOTE: Identical to CVEG(nuc,5,loc), where CVEG has been used to generalize the calculations for different vegetation types.

LIMEIN INIT. CONC. LIMESTONE [mol m^{-3}] Initial concentration of limestone (as $CaCO_3$) in the tailings. Parameter used in the TSOURC modules and calculated using equation (3.3.45) of SENES Vol. 3.

#LOCA LOCATION OF RECEPTOR'S AIR [-]. The segment of the total study area in which the receptor is located (one of eighty) and in which he receives his internal dose from air. A selected parameter defined by the user for a particular run.

LOCF LOCATION OF RECEPTOR'S FISH [-]. The segment of the watershed (one of eight) from which the receptor obtains contaminated fish. A selected parameter defined by the user for a particular run.

LOCV LOCATION OF RECEPTOR'S VEGETABLES [-]. The segment of the total study area (one of eighty) from which the receptor obtains contaminated vegetables. A selected parameter defined by the user for a particular run.

LOCW LOCATION OF RECEPTOR'S WATER [-]. The segment of the watershed (one of eight) from which the receptor obtains contaminated water. A selected parameter defined by the user for a particular run.

LRIVER(n) LENGTH OF RIVER SEGMENT [m]. The length of the reach of river segment "n". Input parameter used in the DOSE module and sampled from:

Constant	(0.0)	n=2,4,7 (lakes)
	(3.0×10^3)	n=1
	(3.5×10^3)	n=3
	(7.0×10^3)	n=5
	(1.3×10^4)	n=6
	(3.0×10^4)	n=8

NOTE: SENES has used the variable LAREA to refer to both lake areas and river lengths. We have kept these parameters separate and used LAREA only for lake areas, LRIVER only for river lengths.

MBAR REPRECIP. BASO4 [mol m^{-2}]. The amount of barite ($BaSO_4$) reprecipitated in the unsaturated zone (per unit area). Intermediate time dependent variable used in the TSOURC modules and calculated using equation (3.10.11) of SENES Vol. 3.

METDIA INTERNAL DOSE (AR) FROM MEAT [µSv a^{-1}]. Internal dose to an average receptor due to ingestion of contaminated meat. Major time dependent output from the DOSE module. No equation given in SENES, but calculated from the sum of all nuclide doses to the receptor from moose and caribou ingestion.

METDIC INTERNAL DOSE (CR) FROM MEAT [μSv a^{-1}]. Internal dose to a critical receptor due to ingestion of contaminated meat. Major time dependent output from the DOSE module. No equation given in SENES, but calculated from the sum of all nuclide doses to the receptor from moose and caribou ingestion.

MEVSV GROUNDSHINE CONVERSION FACTOR [Sv kg s γ-rays^{-1} MeV^{-1} a^{-1}]. Conversion factor from MeV kg^{-1} s^{-1} to Sv a^{-1} taking 1 rad = 1 rem (for γ-rays). Used in the GSHINE module equation (7.13) and defined there as sampled from:

Constant (5. x 10^{-6})

MFLOC FRAC. OF MOOSE LOCAL [-]. The fraction of the annual intake of moose meat that is from local moose. Receptor specific input parameter used in the DOSE module and sampled from:

Constant (1.0) - critical receptor
Constant (0.0) - average receptor

MODULE One or more related processes required to produce one or more calculated variables. The modules referred to here appear as one or more FORTRAN subroutines. Modules used here are based on those noted in Figure 2.1 of SENES Vol. 3 (and which are: TSOURCE, WATEX, GWATER, EROS, LAKEPH, RADON, DUST, AIRDIS, SOIL, GSHINE, VEGCON, VEGEAT and DOSE). They were introduced during the construction of this data dictionary and the data dependency diagrams to help with the understanding of the material in SENES Vol. 3. Although these modules are not directly reflected as high-level bubbles in the data flow diagrams, they are useful in organizing some groups of processes. The modules referred to in this data dictionary, and their defining data flow diagrams (DFDs) or data dependency diagrams (DDDs) are as follows:

AIRDIS - "Calculate Conc. of Contaminants in Air at 80 Receptor Locations and Study Area and Watershed Average Conc." (DFD 2.3)
DOSE - "Calculate Dose" (DFD 4.0)
DUST - "Calculate Ann. Avg. Emission Rate U, Th, Ra, Pb in Dust from Tailings" (DFD 2.1)
EROS - "Calculate Mass Loss from Tailings by Erosion" (DFD 1.6)
FISH - "Calculate Ingestion of Fish Dose" (DFD 4.1.5)
GSHINE - "Calculate Total Groundshine Dose Rate" (DFD 2.5)
GWATER - "Calculate Groundwater Radionuclide Discharge Conc." (DFD 3.1)
LAKEPH - "Calculate pH of Lake n" (DFD 3.2)
RADON - "Calculate Ann. Avg. Emission Rate of Rn Gas from Tailings" (DFD 2.2)
SOIL - "Calculate Radionuclide Conc. in Soil Layers" (DFD 2.4)
TSOURC - "Calculate Source Term Concentrations" (DFD 1.0)
VEGCON - "Calculate Ingest. of Veg. Dose", "Calculate Ingest. of Moose Dose" and "Calculate Ingest. of Caribou Dose" (DFD's 4.1.1, 4.1.2 and 4.1.3)
VEGEAT - "Calculate Ingest. of Moose Dose" and "Calculate Ingest. of Caribou Dose" (DFD's 4.1.2 and 4.1.3)
WATEX - "Calculate Watershed Aqueous Solution Radionuclide Concentrations" (DFD 3.3)

MODOS(nuc) MOOSE DOSE [μSv a^{-1}]. Average annual whole body dose of radionuclide "nuc" (nuc = nat-U, tot-Th, Ra-226, Pb-210) from ingestion of moose meat for a specific location and receptor type. Intermediate time dependent parameter used in the DOSE module and calculated using equation (13.3) of SENES Vol. 3.

MOMIN ANN. INTAKE OF MOOSE [g(wet) a^{-1}]. The average annual intake of moose meat. Receptor specific input parameter used in the DOSE module and sampled from:

Constant (3.95×10^4) - critical receptor
Uniform ($0.0, 3.2 \times 10^3$) - average receptor

MPCH2O PERCENT MOISTURE CONTENT OF TAILINGS [%]. Percent moisture content by weight of the tailings. Input parameter used in the RADON module and sampled from:

Triangular (5, 15, 25)

MSLP USLE EXPONENT [-]. Exponent used in the Universal Soil Loss Equation. Intermediate parameter used in the EROS module and calculated from equations below equation (3.14.3) of SENES Vol. 3.

MSOIL SILT FACTOR [-]. Factor used to account for the clay content of soils when determining erodibility. Intermediate parameter used in the EROS module and calculated from an equation below equation (3.14.4) of SENES Vol. 3.

MU(nuc,band,sla) LINEAR ATTENUATION COEFFICIENT FOR SOIL LAYER [m^{-1}]. The energy dependent attenuation coefficient for a particular soil layer, set equal to the absorption coefficient. Intermediate variable calculated for a particular energy band (band=1,NBAND) for radionulclide chains (nuc=U, Th, Ra (total chain) and Pb, and soil layers (sla=1,NLAYER) in the GSHINE module using equations (7.10) and (7.11) of SENES Vol. 3.

MUD(nuc,band,sla) ATTENUATION PRODUCT [-]. Product of the linear attenuation coefficient and the soil layer thickness. Intermediate variable not specifically defined by SENES, but used in the GSHINE module to simplify equation (7.3). Calculated for all nuclide chains, band energies and soil layers from:

MUD(nuc,band,sla) = MU(nuc,band,sla) x DSOIL(sla).

MUFLSH(band) TISSUE MASS ENERGY ABSORPTION COEFFICIENT [m^2 kg^{-1}]. The mass energy absorption coefficient for tissue at a the energy of a specified energy band. Input parameter used in the GSHINE module and sampled (for all energy bands used) from:

Constant (3×10^{-3})

NBAND NUMBER OF ENERGY BANDS [-]. Number of different energy bands considered in the GSHINE module. Input parameter used in the GSHINE module and sampled from:

Constant (5) (SENES letter 1987-02-03).

NDEC(nucc,band) TOTAL GAMMA RAYS, NUCLIDE [γ-rays kg^{-1} s^{-1}]. Total number of gamma rays per second in a particular energy band from any specified radionuclide decay chain. Used in the GSHINE module.These are sampled from:

Constants (SENES letters, 1986-10-15, 1986-11-04, 1987-02-03):

DECAY CHAIN	1	2	3	4	5
U238 - U234	9.60E+05	0.0	0.0	1.26E+05	0.0
Th232-Pb208	1.45E+05	2.795E+06	1.58E+06	2.27E+06	1.52E+06
Pb210	1.2 E+14	0.0	0.0	0.0	0.0
Ra226(only)	1.46E+12	0.0	0.0	0.0	0.0
Rn222-Pb206	1.46E+12	2.01E+13	1.72E+13	6.23E+12	6.22E+12

The total radium chain is the sum of the Ra226 and Rn222-Pb206 chains. Because of emission of radon from soil, the number of

	decays for groundshine dose calculations must be devived from the values for the two chains using equation (7.8) of SENES Vol. 3. In the DDD's the Ra226 chain is referred to as (Ra°) (radium only), and the value from the calculation for the total radium chain is noted as (Ra).
NLAYER	NUMBER OF SOIL LAYERS [-]. The number of soil layers used in the SOIL and GSHINE modules. The minimum is two if the VEGCON module is used. Sampled from: Constant (2).
NLEN	NUMBER OF SLOPE SEGMENTS [-]. The maximum number of equal-length segments, each less than 400 ft., into which the tailings pile is subdivided for the purpose of calculating erosion losses. Intermediate parameter used in the EROS module, and calculated as the integer part of the expression: ((LENGT / 400) + 1) as discussed on page 3-124 of SENES Vol. 3 and in a letter from SENES (1987-01-13).
NPRCP	NET PRECIPITATION [m a^{-1}]. Net precipitation (accounting for evapotranspiration). Input parameter used in the TSOURC, SOIL and LAKEPH modules and sampled from: Normal (0.4, 0.1, 0.15, 0.65) for DT ≡ Δt = 1 a. NOTE: The value of NPRCP must be sampled separately in each time interval Δt. Even if the time intervals are constant, the value of NPRCP is not. It is a TIME DEPENDENT INPUT PARAMETER. NOTE: The Normal distribution given above is for a single year. If the value of Δt ≠ 1 a, the DISTRIBUTION MUST BE ADJUSTED ACCORDINGLY.
NSUBW	WINTER MONTHS PER YEAR [months a^{-1}]. The number of months per year the surface of the tailings area can be considered to be frozen and/or snow-covered. Input parameter used in the RADON and DUST modules and sampled from: Constant (5)
NU	KINEMATIC VISCOSITY [$ft^2\ s^{-1}$]. The kinematic viscosity for water. Parameter used in the EROS module and sampled from: Constant (1.5×10^{-5}) not as given below equation (3.14.15) of SENES Vol. 3., but (for 7°C) from a SENES letter(1987-01-13).
O2CONC	O_2 CONC. IN AIR [mol m^{-3}]. Concentration of oxygen in air at the surface of the tailings. Input parameter used in the TSOURC module and sampled from: Constant (9.04)
O2DIFF	O_2 DIFFUSIVITY IN TAILINGS [$m^2\ a^{-1}$]. Diffusion coefficient for the diffusion of oxygen through the unsaturated zone in the tailings. Input parameter used in the TSOURC modules and sampled from: Triangular (30, 70, 130)
OF	OCCUPANCY FACTOR [-]. Fraction of the year spent at the receptor site and exposed to inhalation of nat-U, tot-Th, Ra-226 and Pb-210 from dust, and Rn gas. Input parameter used in the DOSE module and sampled from: Triangular (0.4, 0.6, 0.9) - critical receptor Triangular (0.8, 0.9, 1.0) - average receptor NOTE: It is not clear why this parameter is not used when groundshine dose is being calculated.

PAIRDS List of input (sampled) parameters required for the calculation of concentrations of airborne contaminants and consisting of: XDIST, HSRC, FWIND, STAR, AW, BW, RL, ATAIL, WATSHN and WATSHD.

PARAMETER An arbitrary constant or variable so appearing in a mathematical expression that changing it gives various cases of the phenomenon represented (McGraw-Hill Dictionary of Scientific and Technical Terms, 1978). As used here, parameters are input variables to the uranium tailings model, and will be sampled during the stochastic simulation process.

PATMOS List of input (sampled) parameters required for the calculation of concentrations from atmospheric pathways (the AIRDIS + RADON + DUST + SOIL + GSHINE + VEGCON modules), and consisting of the contents of PAIRDS + PDUST + PGSHIN + PRADON + PSOIL + PVGDEP.

PBCF CONVERSION FACTOR MOL TO BQ (PB-210) [Bq mol^{-1}]. Conversion factor used to convert lead-210 concentrations in [mol m^{-3}] to [Bq m^{-3}]. Used inthe TSOURC modules. Defined in equation (3.7.46) of Vol. 3 of the SENES report. PBCF is treated as an input parameter sampled from

Constant (6.3×10^{14})

PBSTI PB-210 ASSOC. PBSO4, UNSAT. PLUS MIX [mol m^{-2}]. The total lead-210 associated with $PbSO_4$ in the unsaturated and mixing zones of the tailings. Intermediate parameter used in the TSOURC modules, and calculated using the equation:

PBSTI = CPBI x FLEAD x (DMIX + DUNSAT).

NOTE: This parameter is used in equation (3.11.18) of SENES Vol. 3, however, no explicit definition is given there or in the referenced section 3.7.4. Also, no computer symbol is noted for this parameter in Table A.3. It is analogous in use (but not in its defining equation) to BASATI. It was defined from an equation:

$$M_{Pb}{}^{\circ} = X_{oPb\text{-}210/PbSO4} \times [PbSO_4]^{\circ} \times (\lambda_w + \lambda_{mix})$$
$$= f_{Pb} \times [Pb\text{-}210_s]^{\circ} \times (\lambda_w + \lambda_{mix})$$

given in a letter from SENES (1986-12-02).

PCHEMS List of input (sampled) parameters required to calculate chemistry parameters (pH, calcium and sulphate concentrations) in the TSOURC module. It consists of FRACGP, XLIME, DUNSAT, FACTCO, DMIX, KPRIME, KSUBSO, O2CONC, O2DIFF, PYRITI, RHOTAL, SULPRD, POROS, FNPRCP, AVPRCP. The variable DT is also included.

PCTHOR MASS % TH [-]. Mass % of thorium (as ThO_2) in the original ore. Input parameter used in the TSOURC modules and sampled from:

Uniform (0.02, 0.04)

PCURAN MASS % U (AS U_3O_8) IN ORE [-]. Mass % uranium (as U_3O_8) in the original ore. Input parameter used in the TSOURC modules and sampled from:

Constant (0.1)

PDOSEI List of input (sampled) parameters required for the calculation of internal dose, and consisting of the contents of PING and PINH.

PDUST List of input (sampled) parameters required for the calculation of Ra emanation in dust at the tailings source (the DUST module) and consisting of: SILT, FPREC, FWINDT, NSUBW, RHOTAL.

P[illegible]M PERCENT ORGANIC [-]. The percentage of organic matter of the tailings. Input parameter used in the EROS module and sampled from:

Constant (0.0)

(SENES letter, 1986-12-02).

PEROS List of input (sampled) parameters required to calculate the mass loss from the tailings pile by erosion (EROS module). It consists

	of ATAIL, CFFM, SILT, THALF, SLOPE, RSOIL, RRAIN, DM, NU, PEROM, BSOIL, CSL, STORM. The variable DT is also included.
PGSHIN	List of input (sampled) parameters required for the calculation of groundshine from a particular decay chain at a receptor site (the GSHINE module) and consisting of: EMFRAC, DSOIL, SPA, RHOS, MEVSV, NBAND, MUFLSH, NDEC, NLAYER and ENERGY.
PGWAT	List of input (sampled) parameters required for the calculation of radionuclide concentrations discharged from groundwater, and consisting of: LAMDA, XRGWAT, POGWAT, AXGWAT, FNPRCP, AVPRCP, ATAIL, SGGWAT, DCGWAT. The variable DT is also included.
PH1	PH LAYER 1 [-]. The pH of solution in the gypsum-depleted layer of the unsaturated zone of the tailings. Time dependent variable used in the TSOURC modules and calculated from equation (3.6.17) if no calcite is present and equation (3.6.18) the presence of calcite. PH1 is equivalent to what SENES calls PH(1).
PH2	PH LAYER 2 [-]. The pH of solution in the gypsum-containing layer of the unsaturated zone of the tailings. Time dependent variable used in the TSOURC modules and calculated from equation (3.6.25) of SENES Vol. 3 for tailings mixed with limestone (INLIME > 0), and from equation (3.6.23) in the absence of $CaCO_3$. PH2 is equivalent to what SENES calls PH(2). NOTE: This pH value is the value required in equations (3.3.65) and following, as the two solids will exist at the boundary at depth DGYP and the pH should be set by them (confirmed by a letter from SENES (1986-11-04)). NOTE: See DDD 1.1.2.8 for several changes to original equations and logic for calculation of PH2.
PH3	PH LAYER 3 [-]. The pH of solution in the mixing layer of the saturated zone of the tailings. Time dependent variable used in the TSOURC modules and calculated from equation (3.6.35) of SENES Vol. 3. PH3 is equivalent to what SENES calls PH(3).
PH4	PH LAYER 4 [-]. The pH of solution in the bottom layer of the saturated zone of the tailings. Time dependent variable used in the TSOURC modules and calculated from equation (3.6.35) of SENES Vol. 3. PH4 is equivalent to what SENES calls PH(4).
PING	List of input (sampled) parameters required to calculate ingestion doses. It consists of DCFGA, AVEGIN, BVEGIN, AFACT, BFACT, AFLOC, BFLOC, LRIVER, LAREA, WATVTC, FMTCM, FIRM, FAIBM, WIRM, MFLOC, MOMIN, DCFGW, FIRC, FMTCC, FAILC, FAISFC, WIRC, CARMIN, CFLOC, WATIN, WFLOC, BIOACF, FISHIN, FFLOC, SHEDAR(n=8), and STDYAR where n=8 is watershed node 8.
PINH	List of input (sampled) parameters required to calculate inhalation doses. It consists of DCFHA, AIRIN, OF, INOCC and EFR.
PLAKPH	List of input (sampled) parameters used in the calculation of the pH of the lakes. It consists of ACTCO, WATCAB, WTSO4B, SHEDAR, ATAIL, LAREA and SDEPTH. The variable DT is also included.
POGWAT	AQUIFER POROSITY [-]. The ratio of the void volume to the total volume for a sandy aquifer. Input parameter used in GWATER and sampled from: Uniform (0.30, 0.36)
POROS	TAILINGS POROSITY $[m^3\ m^{-3}]=[-]$. Fraction of void space in the tailings (porosity). Input parameter used in the TSOURC and RADON modules, and sampled from: Triangular (0.35, 0.40, 0.45) Note: POROS cancels when used in the equations for EBKDFC and

	DIFLEN, and so is an extraneous parameter when used with these parameters. POROS is required, however, in the calculation of WCONC(1,3,3) and elsewhere.
PPBS	List of input (sampled) parameters required to calculate Pb-210 concentrations, in the solid and aqueous phases of the tailings system. It consists of LAMRAD, LAMPB, PBCF, RHOTAL, FLEAD, KSLEAD, FACTCO, KDLEAD, CLEADI, RACF, KFLEAD, DLEADZ, DUNSAT, DMIX, POROS, AVPRCP and FNPRCP. The variable DT is also included.
PRADON	List of input (sampled) parameters required for the calculation of Rn gas emanation at the tailings source (the RADON module), and consisting of: ATAIL, NSUBW, WTSFLX, RNLAM, EMANAT, POROS, MPCH2O and DUNSAT.
PRAS	List of input (sampled) parameters required to calculate radium concentrations in the solid and aqueous phases of the tailings system. It consists of LAMRAD, LAM230, RACF, RHOTAL, FRAD, KSBAR, FACTCO, XRADI, KFBAR, DBARZ, KRAD, DUNSAT, DMIX, POROS, KDRAD, FNPRCP and AVPRCP. The variable DT is also included.
PSOIL	List of input (sampled) parameters required to calculate the concentration of a particular radionuclide at a receptor site (SOIL module) consisting of: SYEAR, DEPVEL, SOILA, RHOS, WC, SOILKD, DSOIL, RHOW, ZMDT, LAMDA and FWAT. The parameter DT is also included.
PSOURC	List of input (sampled) parameters required for the calculation of chemical and radionuclide concentrations (solid and aqueous) in the tailings layers. This consists of the contents of PCHEMS + PUS + PTHS + PRAS + PPBS + PEROS. The variable DT is also included.
PTHS	List of input (sampled) parameters required to calculate thorium concentrations in the solid and aqueous phases of the tailings system. It consists of PCURAN, FT232, PCTHOR, RHOTAL, T230CF, FT230, T232CF, FRACTH, DUNSAT, FACTCO, DMIX. The variable DT is also included.
PUS	List of input (sampled) parameters required to calculate uranium concentrations in the solid and aqueous phases of the tailings system. It consists of FURAN, RHOTAL, PCURAN, FRACU, UCF, PYRITI, DUNSAT, KDUO2, DMIX, POROS, AVPRCP, FNPRCP. The variable DT is also included.
PVGDEP	List of input (sampled) parameters required for the calculation of CVEG (in the VEGCON module), and consisting of DEPVEL, FDEPSF, FDEPED, VEGLAM, DUREXP, YDEN, SPTC and RHOS(2), where the "2" refers to soil layer 2.
PVGEAT	List of input (sampled) parameters used to calculate concentrations of uranium, thorium, lead-210 and radium-226 in moose and caribou meat (VEGEAT module), and consisting of WATVTC, LRIVER, FAIBM, WIRM, FIRM, FMTCM, LAREA, FMTCC, SHEDAR(8), FIRC, WIRC, FAILC, FAISFC and STDYAR.
PWATER	List of input (sampled) parameters required for the calculation of concentrations from water pathways (the GWATER + LAKEPH + WATEX modules), and consisting of the contents of PGWAT + PLAKPH + PWATEX. The variable DT is also included.
PWATEX	List of input (sampled) parameters used in the calculation of concentrations from lake pathways (the WATEX module), and consisting of: WKDU, WKDRA, WKDPB, WATEPS, WTMIXD, WTRHOS, LAMPB, LAMRAD, WSIGS, BURYF, SDEPTH, CURRNT, DIFFC, LAREA, RHOTAL and KDPRIM. The variable DT is also included.

PYRITI	INIT. CONC. OF PYRITE IN TAILINGS [mol m^{-3}]. Initial concentration of pyrite in the tailings. Input (sampled) parameter used in the TSOURC modules and sampled from: Uniform (600., 800.). NOTE(1): PYRITI is the same as PYRITE(1) used by SENES (2): the value of PYRITE(2) at $t=-\Delta t$ as used by SENES is the same as the value of PYRITI
PYRITE	PYRITE CONC. IN TAILINGS [mol m^{-3}]. Concentration of pyrite in tailings at TIME=t. Intermediate parameter used in the TSOURC modules and calculated using equation (3.3.11) of SENES Vol. 3. NOTE: PYRITE is defined as having a minimum value of 1.0×10^{-6} [mol m^{-3}]. NOTE: SENES uses PYRITE(1), PYRITE(2) and PYRITE(3) to represent the values of PYRITE at $time=-\Delta t$, $time=t-\Delta t$, and $time=t$, respectively. NOTE: The initial conditions are PYRITE=PYRITI at $t=0$ and $t=-\Delta t$ (inspection of the UTAP2 code).
Q(nuc)	EMISSION RATE OF RADIONUCLIDE IN DUST FROM TAILINGS SURFACE [Bq s^{-}] Emission rate of radionuclide (nuc= nat-U, tot-Th, Ra-226, Pb-210) in dust from the tailings surface, as a function of time. Intermediate variable calculated in the DUST module. Calculated using equation (4.7) in section 4.2 of SENES Vol. 3.
R(nuc)	RETARDATION FACTOR [-]. A bulk retardation factor for a particular element (Pb, Ra, U, Th). Intermediate variable used in the GWATER module and calculated from equation 9.5 of SENES Vol. 3.
RACF	CONVERSION FACTOR MOL TO BQ (RA-226) [Bq mol^{-1}]. Conversion factor used to convert radium concentrations in [mol m^{-3}] to [Bq m^{-3}]. Used in the TSOURC modules. Defined in equation (3.7.34) of Vol. 3 of the SENES report. RACF is treated as an input parameter sampled from Constant (8.26×10^{12})
RADD(loc)	RN GAS DOSE [µSv a^{-1}]. Average annual whole body dose due to inhalation of radon and its daughter products for a specific location and receptor type. Intermediate time dependent parameter used in the DOSE module and calculated using equation at the bottom of page 13-17 of SENES Vol. 3. NOTE: See comment 154 of Appendix A for a correction to this equation.
RADON	MODULE. All processes required to calculate the Rn gas emanation from the tailings source (see DFD 2.2). The major output from RADON is EMRATE(RN).
RAREA(dis)	AREA of RING dis [m^2]. Annular area of ring dis. Intermediate calculated parameter as deduced from the SENES code. It is calculated as shown in DDD 2.3.7a (BWG, 87-04-06).
RHOS(sla)	BULK DENSITY OF SOIL LAYER [kg m^{-3}]. Dry bulk density of the layer of soil, sla (sla=1,NLAYER). Input parameter used in the SOIL module, and sampled from: Log Normal(129.,1.3, 20., 450.) sla=1 (surface layer) Log Normal(1342.,1.1, 1000., 1800.) sla=2 (subsurface layer)
RHOTAL	TAILINGS BULK DENSITY [g m^{-3}]. Bulk density of the tailings. Input parameter used in the TSOURC modules and sampled from: Normal (1.4×10^6, 0.1×10^6, 1.1×10^6, 1.7×10^6) NOTE: SENES Vol. 3 appears to use the symbols ρ_t and ρ_T interchangeably. Each is defined as RHOTAL, in Table A.3 and Table 3.4, respectively.

RHOW	WATER DENSITY [kg m^{-3}]. The density of water at 20°C. Input parameter used in the SOIL module and sampled from: Constant(998.2)
RL(dis)	RING LIMITS [m]. Radii of the 5 rings, with the first ring extending from RL (01) to RL (02). etc. Input parameter, as deduced from the SENES code, and sampled from: Constant RL(01) = 1000 RL(02) = 3000 RL(03) = 5000 RL(04) = 10000 RL(05) = 20000 RL(06) = 50000
RNDIA	INTERNAL DOSE (AR) FROM RADON [μSv a^{-1}]. Internal dose to an average receptor due to inhalation of radon and its daughters. Major time dependent output from the DOSE module. No equation given in SENES, but calculated from the sum of all nuclide doses to the receptor from radon inhalation.
RNDIC	INTERNAL DOSE (CR) FROM RADON [μSv a^{-1}]. Internal dose to a critical receptor due to inhalation of radon and its daughters. Major time dependent output from the DOSE module. No equation given in SENES, but calculated from the sum of all nuclide doses to the receptor from radon inhalation.
RNFLUX	RN FLUX FROM THE ENTIRE UNSATURATED ZONE [Bq m^{-2} s^{-1}]. Rn-222 flux from the upper ($BaSO_4$ depleted) and lower ($BaSO_4$ enriched) layers of the unsaturated zone, as a function of time. Intermediate time dependent variable calculated in the RADON module. Calculated using equations (4.2 and 4.4) of SENES Vol. 3.
RNFXAV	ANN. AVG. RN FLUX FROM THE ENTIRE UNSATURATED ZONE [Bq m^{-2} s^{-1}]. Rn-222 flux from the upper ($BaSO_4$ depleted) and lower ($BaSO_4$ enriched) layers of the unsaturated zone, as a function of time, but averaged on an annual basis to allow for the period the ground will be frozen and/or covered with snow. Calculated using equation 4.5 of SENES Vol. 3.
RNGMID(dis)	DISTANCE FROM SOURCE TO RECEPTOR [m]. Downwind distance from the tailings source to the receptor. Input parameter used in the AIRDIS module. The distance is the distance to the mid-point between successive rings dividing the study region. In the phase III study five regions were defined and RNGMID was sampled from: Constant RNGMID(1) = 2000 (2) = 4000 (3) = 7500 (4) = 15000 (5) = 35000 NOTE: inspection of the SENES code shows that RNGMID is calculated from RL, as shown in DDD 2.3.3.
RNGMDA(dis)	EFFECTIVE DISTANCE FROM SOURCE TO RECEPTOR [m]. The effective distance from the source to the receptor allowing for the source being an area, not a point source. Not explicitly defined in SENES Vol. 3, but used in the AIRDIS module and calculated from the sum of RNGMID and the virtual distance correction for the source from equation 5.5 of SENES Vol. 3.
RNLAN	RN-222 DECAY CONSTANT [s^{-1}]. Radioactive decay constant for Rn-222. Note that the units of RNLAN are different from the units of the other decay constants; however the appropriate equations have been checked for consistency. Input parameter used in the

	RADON module and sampled from: Constant (2.1×10^{-6})
RRAIN	RAINFALL EROS. FACTOR [100(ft tons $acre^{-1}$)(in hr)]. Rainfall erosivity factor for the tailings pile. Input parameter used in the EROS module and sampled from: Uniform (65., 97.5).
RS	SPACING HYDRAULIC RADIUS [ft]. Hydraulic radius for flow over partially vegetated tailings. Intermediate time dependent parameter used in the EROS module and calculated using an equation (for R_s) on page 3-128 of SENES Vol. 3.
RSOIL	BEDLOAD TRANSPORT EQN. CONST. [ft^2 s^{-1} a^{-1} (units of RRAIN)]. A proportionality constant relating the product of runoff volume and peak discharge to rainfall erosivity. An input parameter used in the bedload transport equation of the EROS module, and sampled from: Uniform ($1.\times10^{-8}$, $1.\times10^{-7}$). Units were obtained from a letter from SENES (1987-01-13).
RTCCA(n)	CA CONCENTRATION PARAMETER FOR NODE N [mol m^{-3}]. Concentration parameter for calcium at watershed node n. Intermediate parameter used in the LAKEPH module and calculated using a modified version of equation 10.2 of SENES Vol. 3. NOTE: The first term in this equation (10.2) gives the concentration at the previous node, the second term the concentration from surface water directly from the tailings. The first term should not be used in the calculation of the concentration at node one. The second term should not be used except for calculation of a concentration at node 1. The third term is needed for all cases (SENES letter 1986-10-15).
RTCS(n)	SO4 CONCENTRATION PARAMETER FOR NODE N [mol m^{-3}]. Concentration parameter for sulphate at watershed node n. Intermediate parameter used in the LAKEPH module and calculated using a modified version of equation 10.3 of SENES Vol. 3. NOTE: The first term in this equation (10.3) gives the concentration at the previous node, the second term the concentration from surface water directly from the tailings. The first term should not be used in the calculation of the concentration at node one. The second term should not be used except for calculation of a concentration at node 1. The third term is needed for all cases (SENES letter 1986-10-15).
S1P	RN ACTIVITY EMANATING FROM THE UPPER UNSAT. ZONE [Bq m^{-3} s^{-1}]. Proportional to the rate of emission of Rn-222 per unit area from the upper ($BaSO_4$ depleted) layer of the unsaturated zone. Intermediate time dependent variable calculated in the RADON module. This equation is adapted from the definition for S_i given near equation 4.1 of Vol. 3 of the SENES report. S1P = CONC(4,1,3) x RNLAN x EMANAT
S2P	RN ACTIVITY EMANATING FROM THE UPPER UNSAT. ZONE [Bq m^{-3} s^{-1}]. Proportional to the rate of emission of Rn-222 per unit area from the lower ($BaSO_4$ enriched) layer of the unsaturated zone. Intermediate time dependent variable calculated in the RADON module. This equation is adapted from the definition for S_i given near equation 4.1 of Vol. 3 of the SENES report. S2P = CONC(4,2,3) x RNLAN x EMANAT
SDEPTH(n)	DEPTH LAKE n [m]. Depth of the lake between nodes (n-1) and n in the watershed. Input parameter used in LAKEPH and WATEX modules

and sampled from:

CONSTANT (0.0) n=1,3,5,6,8 (rivers)
(10.) n=2
(4.) n=4
(5.) n=7

SFLOW SOURCE TERM VOLUME DISCHARGE (SURF. FLOW)[m^3 a^{-1}]. Volume of source term discharge from the reference tailings area. Used in the LAKEPH module and calculated from an equation supplied by SENES (1986-10-15):

SFLOW = ATAIL X NPRCP - VSR

SFLUX SULPHATE FLUX FROM OXD'N OF PYRITE [mol m^{-2} a^{-1}]. Net sulphate flux out of the bottom of the unsaturated zone (and into the mixing zone) due to the oxidation of pyrite and the downward movement of water. Intermediate variable calculated in the TSOURC modules, using equation (3.3.9) of SENES Vol. 3 if there is no limestone in the unsaturated zone (INLIME = 0), and from equation (3.3.46) if INLIME > 0.

SGGWAT SAND SOIL DENSITY [kg m^{-3}]. Ratio of the mass of the bulk soil to the volume it occupies. Input parameter used in GWATER and sampled from:

Normal (2650., 110., 2320., 2980.)

SHEDAR(n) CUM. WATERSHED AREA [m^2]. Cumulative drainage area over the n sub-basins in the watershed. Input parameter used in the LAKEPH and DOSE modules and sampled from:

WTSEG	SHEDAR
1	Constant (15 x 10^6)
2	Constant (20 x 10^6)
3	Constant (32 x 10^6)
4	Constant (38 x 10^6)
5	Constant (70 x 10^6)
6	Constant (120 x 10^6)
7	Constant (140 x 10^6)
8	Constant (400 x 10^6)

SILT SILT CONTENT OF TAILINGS SURFACE [%]. Percentage of particles in the tailings smaller than 75 x 10^{-6} m (or 0.075mm in the definition in EROS). Input parameter used in the EROS and DUST modules and sampled from:

Triangular (10.0, 45.0, 90.0).

The definition is ambiguous in SENES Vol .3, but was confirmed in a letter (1987-01-13) from SENES.

SLOPE TAILINGS SLOPE [-]. Overall percentage slope of the tailings pile. Input parameter used in the EROS module and sampled from:

Constant (1.0).

SLPFAC SEGMENT SLOPE FACTOR [-]. The slope factor in the universal soil loss equation (for any segment). Parameter used in the EROS module and calculated from a revised equation provided by SENES in a letter (1987-01-13).

$$SLPFAC = (0.43 + 0.30 \times SLOPE + 0.043 \times SLOPE^2)/6.613$$

NOTE: See DDD 1.6.3.3 for a corrected version of this equation.

SOFOC See SUFOC.

SOIL MODULE. Process required for calculation of the concentrations of the radionuclides in different layers of the soil at a receptor site as a function of time (see DFD 2.4). The major outputs from SOIL are SOILC and SOILCN.

SOILA SOIL AREA [m^2]. Area of the soil at the receptor site. Input parameter used in the soil module and sampled from:

Constant (1.0)

NOTE: Not explicitly noted by SENES, and required only as part of the unit check for BETAO(nuc,sla) and elsewhere in the SOIL module. It probably cancels out eventually wherever it is used.

SOILC(nuc,loc) RADIONUCLIDE CONC. IN ROOT SOIL LAYER [Bq m^{-3}]. The concentration of the radionuclide (nuc) (nuc= Ra-226, Pb-210, tot-Th, nat-U) in the first subsurface soil layer as a function of time. SOILC is the concentration in dry soil. Used in the VEGCON module and calculated in the SOIL module as SOILCN(nuc,2,loc).

SOILCN(nuc,sla,loc) RADIONUCLIDE CONC. IN SOIL LAYER [Bq m^{-3}]. The concentration of the radionuclide (nuc) (nuc= Ra-226, Pb-210, tot-Th, nat-U) in a particular soil layer "sla (sla=1,NLAYER)" at receptor location "loc" as a function of time. Calculated in the SOIL module from the soil radionuclide activity and the soil layer thickness according to:

SOILCN = ZTOT/(SOILA X DSOIL)

from a letter from SENES (1987-02-03). The factor SOILA is a unit area required to maintain the unit check. SOILCN is used in the GSHINE module and in the VEGCON module (as SOILCN(nuc,2,loc) = SOILC(nuc,loc)).

NOTE: See DDD 2.4.6 for additional comments.

SOILKD(nuc) SOIL KD FOR ELEMENT [m^3 kg^{-1}]. Disrtribution coefficient value for element, nuc, on soil (nuc = uranium, thorium, radium, lead). Parameter used in the SOIL module and sampled from:

Log Uniform(1.3E-4, 7.9E+2)	nuc=uranium
Log Uniform(3.29E-3, 1.5E+2)	nuc=thorium
Log Uniform(5.1E-3, 9.5E+2)	nuc=radium
Log Uniform(1.8E-1, 6.3E+1)	nuc=lead

SPA(nuc) RADIONUCLIDE SPECIFIC ACTIVITY [Bq kg^{-1}]. Specific activity per unit mass of radionuclide. Input parameters used in the GSHINE module (SENES letter 1986-10-15) and sampled from constants:

U	1.23E+07
Th	4.03E+06
Pb	3.00E+15
Ra	3.66E+13

SPACE AVERAGE GRASS SPACING [ft]. The average spacing of grass as vegetation. Intermediate time dependent parameter used in the EROS module and calculated from equation (3.14.19) of SENES Vol. 3.

SPTC(nuc,v) SOIL-PLANT TRANSFER COEFFICIENT [-]. The soil-to-plant transfer coefficients for vegetation types v=1,2,3,4,5 (above-ground and below-ground vegetables, summer forage, browse and lichen). This is the ratio of the activity (Bq g^{-1}) plant (wet weight) per unit activity (Bq g^{-1}) in the (first subsurface) soil layer (dry weight). Input parameters used in the VEGCON module and sampled from:

LOG NORMAL	(6.08×10^{-4}, 8.90, 7.67×10^{-6}, 7.00×10^{-3})	v=1	U-nat
	(4.20×10^{-3}, 9.00, 5.19×10^{-5}, 3.40×10^{-1})		Th-tot
	(4.00×10^{-3}, 9.00, 4.94×10^{-5}, 3.24×10^{-1})		Pb-210
	(8.47×10^{-3}, 10.3, 8.03×10^{-5}, 8.93×10^{-1})		Ra-226
	(3.17×10^{-4}, 3.93, 2.06×10^{-5}, 4.89×10^{-3})	v=2	U-nat
	(4.20×10^{-3}, 4.00, 2.62×10^{-4}, 6.72×10^{-2})		Th-tot
	(4.00×10^{-3}, 4.00, 2.50×10^{-4}, 6.40×10^{-2})		Pb-210
	(2.65×10^{-3}, 4.52, 1.29×10^{-4}, 6.60×10^{-2})		Ra-226

(6.60×10^{-3}, 8.91, 8.31×10^{-5}, 5.24×10^{-1}) v=3,4 U-nat
(2.23×10^{-2}, 9.50, 2.47×10^{-4}, 2.01) Th-tot
(2.16×10^{-2}, 3.55, 1.71×10^{-3}, 2.71×10^{-1}) Pb-210
(2.11×10^{-1}, 3.63, 1.87×10^{-3}, 2.39×10^{-1}) Ra-226

CONSTANT (0.0) U-nat, Th-tot, Pb-210, Ra-226 v=5

NOTE: In SENES Vol. 3
SPTC(1)=SPTCAV
SPTC(2)=SPTCBV
SPTC(3)=SPTCSF
SPTC(4)=SPTCB
SPTC(5)=SPTCL (this last name being incorrectly noted as SPTCB(i) in Table 8.5 (SENES letter of 1986-12-02).

The generic parameter SPTC(nuc,v) has been used in the DDD's in the interests of clarity.

SSTAR HYP. SO4 IN MIXING LAYER NO GYP. [mol m^{-3}] Hypothetical concentration of sulphate in the mixing layer if no gypsum were present, calculated for times after gypsum depletion of the unsaturated layer but before gypsum is totally depleted from the mixing layer. Time dependent variable used in the TSOURC modules and calculated from equation (3.4.8) of SENES Vol. 3.

STAR ANNUAL AES WIND AND STABILITY DATA. Annual AES wind and stability data (STAR data) from the Gore Bay weather station for a twenty year period. Input data used in the AIRDIS module.

STDYAR STUDY AREA [m^2]. The total area under study, taken to be given by a circle with radius 50km (SENES Vol. 3, Fig. 2-2 and 10-1). Used in the DOSE module. Input parameter (calculated by considering a circle with radius 5×10^4 [m]) sampled from:

Constant (7.854×10^9).

STORM MAX.24-HR RAINFALL [mm d^{-1}]. The maximum 24-hour rainfall in a two year return period. Input parameter used in the EROS module and sampled from:

Uniform(36,48).

NOTE: Supplied by SENES in a letter (1987-01-13).

SUFOC(nuc) CONC. OF RADIONUCLIDE IN SUMMER FORAGE VEGETATION [Bq g^{-1}(wet weight)]. Average annual concentration of radionuclide (nuc) in summer forage vegetation due to foliar retention of the radionuclide deposited from dust in the air and to root uptake. Values are calculated as a function of time and location. Variable calculated in the VEGCON module and used in the DOSE module. Calculated using equation (8.1) of SENES Vol. 3.

NOTE: Incorrectly given as SOFOC in Table 12.1 of SENES Vol. 3.

NOTE: Identical to CVEG(nuc,3,loc), where CVEG has been used to generalize the calculations for different vegetation types.

SULPRD SULPHATE PRODUCTION RATE [mol g^{-1} a^{-1}]. Sulphate production rate. Input parameter described in Chapter 3 of SENES Vol. 3. Sampled from:

Lognormal (1.4×10^{-6}, 1.5, 0.4×10^{-6}, 4.2×10^{-6})

NOTE: The assumption is made that the symbol R_s in SENES Vol. 3, with and without the bar above the symbol, has the identical meaning.

SUMBAR SUM DISSOLVED RA [mol m^{-2}]. Cumulative sum of radium inputs to the mixing zone to TIME=t. Intermediate time dependent parameter used in the TSOURC modules, and calculated using equation (3.10.35) of SENES Vol. 3. The initial condition is SUMBAR=0 at TIME=$-\Delta t$ (SENES letter 1987-02-03).

NOTE:The dimensions vary for the terms in equation (3.10.35). There are two different parameters here, both referred to as $[Ra]_{in}$. The term on the LHS of equation (3.10.35) corresponds to SUMBAR in Table A.3, however it should have units of $[\text{mol m}^{-2}]$ for comparison with M_{Ra}° in equation (3.10.36). The summation is not really over $[Ra]_{in}$, but of terms like that on the RHS of equation (3.10.35). (SENES agrees, 1986-12-02)

SUMPB SUM DISSOLVED PB-210 $[\text{mol m}^{-2}]$. Cumulative sum of lead-210 inputs to the mixing zone to TIME=t. Intermediate time dependent parameter used in the TSOURC modules, and calculated using equation (3.11.17) of SENES Vol. 3.

NOTE:The dimensions vary for the terms in equation (3.11.17). There are two different parameters here, both referred to as $[Pb]_{in}$. The term on the LHS of equation (3.11.17) corresponds to SUMPB in Table A.3, however it should have units of $[\text{mol m}^{-2}]$ for comparison with M_{Pb}° in equation (3.11.18). The summation is not really over $[Pb]_{in}$, but of terms like that on the RHS of equation (3.11.17). (SENES agrees, 1986-12-02).

NOTE: SUMPB=0 at TIME=$-\Delta t$ (inspection of the UTAP2 code).

SUNCOM CONC. UNCOMP. SO4 BOTTOM UNSAT. ZONE $[\text{mol dm}^{-3}]$. Total concentration of uncomplexed sulphate ion at the bottom of the unsaturated zone. Intermediate time dependent parameter used in the TSOURC modules and calculated using equation (3.3.41) of SENES Vol. 3. Noted in Table A.3 of the SENES Vol. 3 as being denoted by "several" symbols in their computer programs.

SUS(eseg) SEDIMENT AVAILABLE FOR TRANSPORT $[\text{lb ft}^{-1}\text{ a}^{-1}]$. Sediment available for transport in segment "eseg" of the tailings pile. Intermediate time dependent parameter not explicitly defined in SENES Vol. 3, but used in the EROS module and calculated from a modified version of equation (3.14.20) (letter, 1987-01-27).

NOTE: See DDD 1.6.3.6 for more recent comments.

SWCONC(nuc,sla) AVG. AQ. RADIONUCLIDE CONC. IN SOIL LAYER $[\text{Bq m}^{-3}]$. The concentration of the radionuclide (nuc) (nuc=Ra-226, Pb-210, (Th-232 + Th-230), natural uranium) partitioned into the water in equilibrium with a soil layer (sla) at a time that is the average of t and $(t-\Delta t)$. Time dependent intermediate variable calculated in the SOIL module.

NOTE: Values for LAMDA(nuc) are not supplied for the same thorium and uranium isotopes used in the calculations of AIRC, and according to SENES (letter, 1986-12-11) the differences were considered by SENES to be unimportant to the current model.

SYEAR SECONDS IN A YEAR $[\text{s a}^{-1}]$. The number of seconds in a year. Input parameter used in the SOIL module to convert DEPVEL from $[\text{m s}^{-1}]$ to $[\text{m a}^{-1}]$. Not given in the SENES documents but sampled from

Constant (3.1536×10^{7})

NOTE: Value comfirmed in SENES letter of 1986-12-02.

T230CF TH-230 CONVERSION FACTOR $[\text{Bq mol}^{-1}]$. Conversion factor used to convert ^{230}Th concentrations in $[\text{mol m}^{-3}]$ to $[\text{Bq m}^{-3}]$. Used in the TSOURC modules and treated as an input parameter sampled from:

Constant (1.65×10^{11})

T230D CONC. DISS. TH-230 IN UNSAT. ZONE $[\text{mol m}^{-3}]$. The concentration of dissolved Th-230 to TIME=t in the unsaturated zone. Intermediate parameter used in the TSOURC modules and calculated using equation (3.9.6).

T230IS	INIT. CONC. INSOL. TH-230 [mol m^{-3}]. Initial concentration of insoluble Th-230 in the tailings. Intermediate parameter used in the TSOURC modules and calculated using equation (3.7.21) of SENES Vol. 3.
T230S	CONC. SOLID TH-230 IN UNSAT. ZONE [mol m^{-3}]. The solid phase concentration of Th-230 in the unsaturated zone. Intermediate parameter used in the TSOURC modules and calculated using equation (3.9.7) of SENES Vol. 3.
T230SO	INIT. CONC. SOLU. TH-230 [mol m^{-3}]. Initial concentration of soluble Th-230 in the tailings. Intermediate parameter used in the TSOURC modules and calculated using equation (3.7.19) of SENES Vol. 3.
T232CF	TH-232 CONVERSION FACTOR [Bq mol^{-1}]. Conversion factor used to convert ^{232}Th concentrations in [mol m^{-3}] to [Bq m^{-3}]. Used in the TSOURC modules and treated as an input parameter sampled from: Constant (9.35 x 10^5)
T232D	CONC. DISS. TH-232 IN UNSAT. ZONE [mol m^{-3}]. The total concentration of Th-232 dissolved in the unsaturated zone to TIME=t. Intermediate parameter used in the TSOURC modules and calculated using equation (3.9.5).
T232IS	INIT. CONC. INSOL. TH-232 [mol m^{-3}]. Initial concentration of insoluble Th-232 in the tailings. Intermediate parameter used in the TSOURC modules and calculated using equation (3.7.22) of SENES Vol. 3.
T232S	CONC. SOLID TH-232 IN UNSAT. ZONE [mol m^{-3}]. The solid phase concentration of Th-232 in the unsaturated zone. Intermediate time dependent parameter used in the TSOURC modules and calculated using equation (3.9.8) of SENES Vol. 3.
T232SO	INIT. CONC. SOLU. TH-232 [mol m^{-3}]. Initial concentration of soluble Th-232 in the tailings. Intermediate parameter used in the TSOURC modules and calculated using equation (3.7.20) of SENES Vol. 3.
TAREA	TOTAL AREA OF RINGS [m^2]. Total area of the 5 rings. Intermediate calculated parameter as deduced from the SENES code, and probably a replacement for STDYAR. It is calculated as shown in DDD 2.3.7A (BWG, 87-04-06).
TCSOIL(eseg)	SEGMENT BEDLOAD TRANSPORT CAPACITY[lb ft^{-1} a^{-1}]. Bedload transport capacity of the tailings for the jth segment. Intermediate time dependent parameter used in the EROS module and calculated using equation (3.14.8) of SENES Vol. 3. The equation for "x" was provided in a letter frpm SENES (1987-01-13).
TH(n)	RADIOACTIVE HALF-LIFE [a]. Half-life of radionuclide (n) (n= U-238, Th-232, Pb-210, Ra-226). Input parameters used by SENES in the GWATER module. Directly related to the LAMDA parameters in the SOIL module by: LAMDA = ln(2) / TH. NOTE: ln2 / TH(U-238) $\neq$ LAMDA(U-238) (minor difference) NOTE: LAMDA is really the required parameter in the GWATER module, and used there instead of TH.
THALF	REVEG. HALF LIFE [a]. The time required for half the bare tailings area to become revegetated (provided pH > 4). Input parameter used in the EROS module and sampled from: Uniform (10., 20.).
THDISM	CONC. TOTAL TH DISS. MIXING LAYER [mol m^{-3}]. The concentration of total thorium (Th-230 and Th-232) that has dissolved in the mixing

	layer of the saturated zone to TIME=t. Intermediate parameter used in the TSOURC modules and calculated using equations (3.9.17) and (3.9.18) of SENES Vol. 3. THDISM can take on negative values to reflect precipitation in the mixing layer. NOTE: THDISM=0.0 at TIME=$-\Delta t$ and TIME=0 are the initial conditions (SENES letter, 1987-01-27 and inspection of the UTAP2 code).
THDISS	CONC. TOTAL TH DISS. [mol m^{-3}]. The concentration of total thorium (Th-230 and Th-232) that has dissolved in the unsaturated zone to TIME=t. Intermediate parameter used in the TSOURC modules and calculated using equation (3.9.4) of SENES Vol. 3 if THDISS < THSOL, or set equal to THSOL if the calculated value of THDISS $\geq$ THSOL (inferred from the text near equation (3.9.12) of SENES Vol. 3). NOTE: THDISS=0.0 at TIME=$-\Delta t$ and TIME=0 are the initial conditions (SENES letter, 1987-01-27 and inspection of the UTAP2 code).
THORCF	WT. TH CONVERS. FACTOR [Bq mol^{-1}]. The weighted liquid phase thorium conversion factor for solutions containing both Th-230 and Th-232. Intermediate conversion factor used in the TSOURC modules and calculated using equation (3.7.31) of SENES Vol. 3.
THORDC	LOG APPAR. SOL. PROD. TH(OH)4 [-]. The averaged (apparent) value of the logarithm (base 10) of the solubility product of a mixture of amorphous and crystalline thorium hydroxide. Intermediate parameter calculated in the TSOURC modules and calculated using equation (3.9.3) of SENES Vol. 3.
THSOL	INIT. CONC. TOTAL SOLU. TH [mol m^{-3}]. The initial concentration of total soluble thorium (Th-230 + Th-232) in the tailings. Intermediate parameter used in the TSOURC modules and calculated using equation (3.7.23) of SENES Vol. 3
TIME	TIME [a]. Independent variable, implicitly included in the calculation of most variables, and explicitly appearing in the calculation of some variables. Used in many of the modules. Table 5.1 of SENES Vol. 3 suggests that TIME ranges from 0 to 500 in steps (DT) of 10 a. Major output variables in the tailings submodel are output every 50 a.
TRSED	FRACT. TRAPPED SED. [-]. Fraction of the suspended sediment trapped by vegetation. Intermediate time dependent parameter used in the EROS module and calculated using equation (3.14.15) of SENES Vol. 3. even if there is no vegetation on the tailings. (SENES letter, 1987-01-27). Also, equation (3.14.15) has been modified (SENES letters, 1987-01-27 and 1987-02-04).
TSOIL	TRANSPORT. SOIL (BEDLOAD) [lb s^{-1} ft^{-5}]. A parameter representing the transportivity of soil particles in bedload transport. Used in the EROS module and calculated from equation (3.14.9) of SENES Vol. 3.
TSOURC	MODULES. All processes required to calculate the tailings source terms which are used in other modules (see DFD 1.0). Usually referred to in the plural, since the calculation processes in TSOURC are very complex and long. The EROS module could be considered as part of TSOURC, but has been separated out because the equations in EROS are substantially different from other equations in TSOURC. The major variables produced by TSOURC include AEXPT, CONC, DBAR, IGRA, IGPB, X230LA, X232LA, X232SA and WCONC.
TVEG	TIME VEG. BEGINS [a]. The time at which (re)vegetation of the tailings pile begins. Intermediate parameter used in the EROS module, and assigned according to the time at which PH1 becomes ≥ 4

(SENES Vol. 3, pg. 3-123,124).
NOTE: See DDD 1.6.1.7 for additional comments.

UCF CONVERSION FACTOR MOL TO BQ (NAT-U) [Bq mol^{-1}]. Conversion factor used to convert natural uranium concentrations in [mol m^{-3}] to [Bq m^{-3}]. Used in the TSOURC modules and defined in equation (3.7.5) of Vol. 3 of the SENES report. UCF is treated as an input parameter sampled from

Constant ($5.95x10^6$)

UNSAT. ZONE: Abbreviation used to designate the unsaturated portion of the tailings pile. As shown in Figure A.1 of Appendix A in SENES Volume 3, the unsaturated zone consists of an upper (gypsum-depleted) layer of depth = DEPTH1 and radium concentration = RACON1, and a lower (gypsum-enriched) layer of depth = DEPTH2 and radium concentration = RACON2. Precipitation falling on the surface of the tailings passes through the unsaturated zone to the saturated zone below. (The saturated zone consists of a mixing layer and other unspecified layers.) Note: the term gypsum-depleted is somewhat confusing; gypsum-free would be more consistent with the model of the unsaturated zone.

UPYRI INIT. CONC. U3O8 ASSOC. WITH PYRITE [mol m^{-3}]. Initial concentration of U_3O_8 associated with pyrite in the tailings. Intermediate parameter used in the TSOURC modules and calculated from equation (3.7.6) of SENES Vol. 3.

UWIND(dir,st) MEAN WIND SPEED, SOURCE TO RECEPTOR [m s^{-1}]. Mean annual wind speed in a particular direction "dir", and of a particular stability class, "st". Variable calculated and used in the AIRDIS module. Calculated from STAR data for Gore Bay using an equation supplied in a letter from SENES (1986-11-04):

[1.50 x FWIND(dir,st,1,n) + 2.46 x FWIND(dir,st,2,n)
4.47 x FWIND(dir,st,3,n) + 6.93 x FWIND(dir,st,3,n)
9.61 x FWIND(dir,st,5,n) + 12.52 x FWIND(dir,st,6,n)]/FWIND2

using the definition of FWIND2 from the same letter.
NOTE: UWIND has a minimum value of 0.5 (inspection of the UTAP2 code).

V1(nuc,n) V1 PARAMETER USED IN WATEX [a^{-1}]. Intermediate parameter used in the calculation of WATRW and WATRS in the WATEX module. This time dependent parameter is defined in an equation below equations (10.32) and (10.33) in SENES Vol. 3.

V2(nuc,n) V2 PARAMETER USED IN WATEX [a^{-1}]. Intermediate parameter used in the calculation of WATRW and WATRS in the WATEX module. This time dependent parameter is defined in an equation below equations (10.32) and (10.33) in SENES Vol. 3.

VARIABLE A quantity (or a symbol representing a quantity) that may assume any one of a set of values (Webster's Ninth New Collegiate Dictionary, 1983). As used here, variable includes input (sampled) parameters (such as NPRCP), calculated variables (such as RACON1), output variables (such as TDOSE), and input independent variables (such as TIME and DT).

VDISP(dis,st) VERTICAL DISPERSION COEFFICIENT [m]. Vertical dispersion coefficient used in the sector-averaged Gaussian plume model for the dispersion of contaminants in the atmosphere. Variable (function of distance (dis) and stability class (st)) calculated and used in the AIRDIS module. Calculated using equations and parameters given in Table 5.2 and equation (5.6) of SENES Vol. 3.

VEGCON	MODULE. All processes required to calculate the concentrations of Ra-226 in edible vegetables due to foliar retention of Ra-226 deposited from air. The major output from VEGCON are the radionuclide concentrations in different types of vegetation (AVEGC, BVEGC, SUFOC, BRWSC, LICHC). In the final specifications (see Appendix B), VEGCON does not appear as a separately-distinguishable module. Elements of VEGCON appear in DFD's 4.1.1, 4.1.2 and 4.1.3, and these diagrams produce the major output variables VEGD, CARDOS and MODOS.
VEGD(nuc,loc)	INGEST.OF VEG. DOSE [μSv a^{-1}]. The average annual whole body dose due to ingestion of above- and below-ground vegetables for radionuclide nuc (nuc=natural uranium, total thorium, Ra-226 and Pb-210). Intermediate time-dependent variable used in the DOSE module and defined in equation (13.1) in SENES Vol. 3:)
VEGDIA	INTERNAL DOSE (AR) FROM VEGETABLES [μSv a^{-1}]. Internal dose to an average receptor due to ingestion of contaminated vegetables. Major time dependent output from the DOSE module. No equation given in SENES, but calculated from the sum of all nuclide doses to the receptor from vegetable ingestion.
VEGDIC	INTERNAL DOSE (CR) FROM VEGETABLES [μSv a^{-1}]. Internal dose to a critical receptor due to ingestion of contaminated vegetables. Major time dependent output from the DOSE module. No equation given in SENES, but calculated from the sum of all nuclide doses to the receptor from vegetable ingestion.
VEGEAT	MODULE. All processes required to calculate the internal dose due to ingestion of caribou and moose that have fed on contaminated vegetation (see DFD's 4.1.2 and 4.1.3). Major output variables produced by VEGEAT are CARDOS and MOSDOS.
VEGLAM(v)	WEATHERING LOSS DECAY RATE [s^{-1}]. 'Decay' constant accounting for weathering loss in vegetation types v=1,2,3,4,5 (above-ground and below-ground vegetables,summer forage, browse and lichen). Input parameters used in the VEGCON module and sampled from: Uniform (2.9×10^{-7}, 1.2×10^{-6}) (v=1,2,3,4) Uniform (1.5×10^{-9}, 4.4×10^{-9}) (v=5)
VEL	FLOW VELOCITY THROUGH GRASS [ft s^{-1}]. Flow velocity through grass calculated as a function of tailings slope. Intermediate time dependent parameter used in the EROS module and calculated from equations (3.14.17) and (3.14.18) of SENES Vol. 3.
VELRAT	VELOC. RATIO (BEDLOAD) [-]. Velocity ratio used in the bedload transport capacity equation. Intermediate parameter used in the EROS module and calculated from equation 3.14.13 of SENES Vol. 3.
VS	SETTLING VELOCITY [ft s^{-1}]. Settling velocity of silt- and clay-size particles. Intermediate parameter used in the EROS module and calculated using equation (3.14.16) of SENES Vol. 3.
VSR	VOLUMETRIC SEEPAGE [m^3 a^{-1}]. Volumetric seepage rate through the aquifer assumed equal to the average tailings seepage rate. Variable used in the GWATER and LAKEPH modules and calculated using equation 9.3 of SENES Vol. 3.
WATAVG(nuc)	AVG. CONC. IN WATERSHED [Bq m^{-3}]. The average concentration of radionuclide "nuc" (nuc = U-nat, Th-tot, Ra-226, Pb-210) along the edge of lakes and rivers in the watershed. Intermediate time dependent parameter used in the DOSE module and calculated from equation (11.4) of SENES Vol. 3.
WATC(7,n)	see WATCS(n)
WATC(8,n)	see WATCCA(n)

WATC(nuc,n) CONCENTRATION OF RADIONUCLIDE IN WATER AT WATERSHED NODE N [Bq m^{-3}]. Concentration of radionuclide (nuc = nat-U, tot-Th, Ra-226, Pb-210) in the aqueous phase at node n of the watershed. Time dependent variable calculated in the WATEX module and used in the DOSE and FISH modules. Calculated using equation (10.9 (river nodes)), and (10.31 (lake nodes)) of SENES Vol. 3.
NOTE: The equation (10.9) must be modified as it includes both the source concentration and the concentration of the radionuclide at node (n-1). The parallel modification of equations (10.2) and (10.3) has been discussed in a letter from SENES (1986-10-15).

WATCAB BACKGROUND CALCIUM CONCENTRATION [mol m^{-3}]. The natural background calcium concentration level in freshwater flow. Input parameter used in the LAKEPH module and sampled from:
Constant (0.1)

WATCCA(n) CA CONCENTRATION AT NODE N [mol m^{-3}]. Concentration of calcium in the aqueous phase at node n in the watershed. Based on the concentration at the previous node (or from groundwater and the mixing zone) and from background levels. Intermediate time dependent variable calculated in the LAKEPH module. Calculated using equation (10.5) of SENES Vol. 3. For the first node the concentration is:

$$\text{WATCCA(1)} = \frac{[\text{WCONC(8,3,3)} \times \text{SFLOW} + \text{WATCAB} \times (\text{FLOWQ(1)}-\text{SFLOW})]}{\text{FLOWQ(1)}}$$

i.e., the groundwater concentration (from WCONC(8,4,3)) is not considered separately (SENES letter, 1987-02-03).
NOTE: SENES uses WATC(8,n) for this variable.
NOTE: See also DDDs 3.2.5, 3.2.5A and 3.2.6 for ammended logic used to calculate this variable.

WATCS(n) SO4 CONCENTRATION FOR NODE N [mol m^{-3}]. Concentration of sulphate in the aqueous phase at node n in the watershed. Based on the concentration at the previous node (or from groundwater and the mixing zone) and from background levels. Intermediate time dependent variable calculated in the LAKEPH module. Calculated using equation (10.5) of SENES Vol. 3. For the first node the concentration is:

$$\text{WATCS(1)} = \frac{[\text{WCONC(7,3,3)} \times \text{SFLOW} + \text{WTSO4B} \times (\text{FLOWQ(1)}-\text{SFLOW})]}{\text{FLOWQ(1)}}$$

i.e., the groundwater concentration (from WCONC(7,4,3)) is not considered separately (SENES letter, 1987-02-03).
NOTE: SENES uses WATC(7,n) for this variable.
NOTE: See also DDDs 3.2.5, 3.2.5A and 3.2.6 for ammended logic used to calculate this variable.

WATD(nuc,loc) INGEST. OF D.W. DOSE [μSv a^{-1}]. Average annual whole body dose of radionuclide "nuc" (nuc = nat-U, tot-Th, Ra-226, Pb-210) from ingestion of water from the watershed for a specific location and receptor type. Intermediate time dependent parameter used in the DOSE module and calculated using equation (13.4) of SENES Vol. 3.

WATDIA INTERNAL DOSE (AR) FROM WATER [μSv a^{-1}]. Internal dose to an average receptor due to ingestion of contaminated water. Major time dependent output from the DOSE module. No equation given in SENES, but calculated from the sum of all nuclide doses to the receptor from water ingestion.

WATDIC INTERNAL DOSE (CR) FROM WATER [μSv a^{-1}]. Internal dose to a critical receptor due to ingestion of contaminated water. Major time dependent output from the DOSE module. No equation given in SENES, but calculated from the sum of all nuclide doses to the receptor from water ingestion.

WATEPS SEDIMENT POROSITY [-]. The volume fraction of liquid in the sediment (sediment porosity). Input parameter used in the WATEX module and sampled from:

Triangular (0.83, 0.94, 0.97)

WATEX MODULE. All processes required to calculate radionuclide concentrations in water at the various watershed node (see DFD 3.3). The major output is WATC(nuc,n) (nuc=nat-U, tot-Th, Ra-226, Pb-210).

WATIN ANN. INTAKE OF WATER [m^3 a^{-1}]. Average annual intake of water. Input parameter used in the DOSE modules and sampled from:

Constant (0.6)

The value is assumed to be the same for both critical and average receptors.

WATKL(n) MASS TRANSFER COEFFICIENT, LAKE [m a^{-1}]. Mass transfer coefficient of the radionuclides into the lake water column from the sediment in the lake between nodes (n-1) and n. Intermediate parameter calculated in the WATEX module from equations 10.15 and 10.16 (see also pg. 10-23) of SENES Vol. 3.

WATPH(n) PH OF LAKE [-]. pH of the lake between nodes (n-1) and n, as a function of time. Variable calculated in the LAKEPH module, used in the WATEX module, and a major output of the tailings submodel. Calculated using equation (10.8) of SENES Vol. 3.

WATRS(nuc,n) QUANTITY OF RADIONUCLIDE IN LAKE SEDIMENT EXCH. ZONE [Bq]. Radionuclide activity in the lake sediment exchange zone of lake n (nuc=nat-U, tot-Th, Ra-226, Pb-210). WATRS and WATRW are intermediate time dependent variables calculated in the WATEX module, and are calculated from the pair of coupled finite difference equations given in equations (10.32) and (10.33) in SENES Vol. 3. The initial conditions are assumed to be WATRW = WATRS = 0 at TIME = $-\Delta t$.

WATRW(nuc,n) QUANTITY OF RADIONUCLIDE IN LAKE WATER COL.[Bq]. Radionuclide activity in the water column of lake n (nuc=nat-U, tot-Th, Ra-226, Pb-210). WATRS and WATRW are intermediate time dependent variables calculated in the WATEX module, and are calculated from the pair of coupled finite difference equations given in equations (10.32) and (10.33) in SENES Vol. 3. The initial conditions are assumed to be WATRW = WATRS = 0 at TIME = $-\Delta t$.

WATSHD(i) WATERSHED AREA LOCATIONS [-]. The specific portions of the study area that comprise the watershed. User specified parameters used in the AIRDIS module and elsewhere to obtain watershed average contamination values. The locations used in the SENES Phase III study are denoted by dir = 1-->16 (direction, N=1, NNE=2 ...) and dis 1-->5 (distance, see RNDDIS(dis)). The watershed locations are locations that contain watershed nodes, and are denoted by:

WATSHD(1)	dir=11	dis=1
(2)	10	2
(3)	9	3
(4)	9	4
(5)	9	5

NOTE: The definition of the watershed area was supplied by SENES in a letter (1986-12-11).

WATSHN NUMBER WATERSHED LOC. [-]. The number of specific portions (direction and distance sections) in the watershed area. User specified parameter used in the AIRDIS module but not specifically noted by SENES.

WATVTC(nuc) WATER AQ. VEG. XFR COEFF [Bq g^{-1}(wet) Bq^{-1} m^3]. The water-to-aquatic vegetation tranfer coefficient for nuclide "nuc" (nuc = nat-U, tot-Th, Pb-210 and Ra-226). Input parameter used in the DOSE module and sampled from:

Lognormal (1.5×10^{-5}, 5.5, 1.0×10^{-6}, 7.0×10^{-4}) nuc = U-nat
(1.1×10^{-5}, 6.8, 1.0×10^{-6}, 1.6×10^{-4}) nuc = Th-tot
(4.5×10^{-5}, 2.9, 1.0×10^{-5}, 3.3×10^{-4}) nuc = Ra-226
(1.3×10^{-4}, 2.0, 4.0×10^{-5}, 4.3×10^{-4}) nuc = Pb-210

WATWS QUANTITY OF RADIONUCLIDE IN LAKE SEDIMENT [Bq]. Radionuclide activity in exchangeable lake sediment as a function of time. WATRS and WATRW are intermediate variables calculated in the WATEX module, and are calculated from the pair of coupled finite difference equations given in equations (10.34) and (10.35) in SENES Vol. 3. The initial conditions are assumed to be WATRW = WATRS = 0 at TIME = $-\Delta t$.

WC(sla) WATER CONTENT OF SOIL LAYER [-]. The water content of the layer, sla, (sla=1,NLAYER) of the soil (kilograms water per kilogram soil). Used in the SOIL module and sampled from:

Uniform(0.75, 1.4) sla=1 (surface soil layer)
Log Normal(0.13, 1.4, 0.05, 3.6) sla=2 (subsurface layer)

WCARC(nuc) WATER - CARIBOU CONC. [Bq g^{-1}(wet)]. Concentration of the radionuclide "nuc" in caribou flesh due to the water pathway (nuc = U-nat, Th-tot, Ra-226, Pb-210). Time dependent parameter used in the DOSE module and calculated from equation (12.2) of SENES Vol. 3.

WCONC(1,2,3) AQ. U IN UNSAT. ZONE [Bq m^{-3}]. The concentration of uranium in the aqueous phase at the bottom of the unsaturated zone. Intermediate time dependent variable calculated in the TSOURC modules. Calculated using equations (3.7.8) and (3.8.2) in SENES Vol. 3. NOTE: Equation (3.8.2) would give the concentration in [mol m^{-3}], and an additional factor of UCF is required to convert the concentration to units of [Bq m^{-3}].

WCONC(1,3,3) AQ. U IN MIXING ZONE [Bq m^{-3}]. The concentration of uranium in the aqueous phase in the mixing zone. Major time dependent output from the TSOURC modules; used in the WATEX module. Calculated using equations (3.7.9) and (3.8.4) in SENES Vol. 3. NOTE: Equation (3.8.4) gives the concentration in whatever units are attributed to WCONC(1,2,3). See WCONC(1,2,3).

WCONC(1,4,3) AQ. U IN BOTTOM LAYER [Bq m^{-3}]. The concentration of uranium in the aqueous phase in the bottom layer of the tailings. Major time dependent output from the TSOURC modules; used in the WATEX module. Calculated using equations (3.7.10) and (3.8.5) in SENES Vol. 3.
NOTE: Equation (3.8.5) gives the concentration in whatever units are attributed to WCONC(1,3,3) and WCONC(1,2,3). See WCONC(1,2,3).

WCONC(1,j,2),(j=2,3,4) as WCONC(1,j,3) above, but for TIME=t-Δt rather than TIME=t

WCONC(2,2,3) AQ. TH IN UNSAT. ZONE [Bq m^{-3}]. The concentration of thorium in the aqueous phase at the bottom of the unsaturated zone. Intermediate time dependent variable calculated in the TSOURC modules. Calculated using equation (3.9.1) in SENES Vol. 3. A maximum value of

$$\text{WCONC}(2,2,3) = 5 \times 10^{-5} \times 10^{3} \times \text{THORCF [Bq m}^{-3}]$$

is assigned. If THDISS $\geq$ THSOL, WCONC(2,2,3)=0 using equation (3.9.12)

WCONC(2,3,3) AQ. TH IN MIXING LAYER [Bq m^{-3}]. The concentration of thorium in the aqueous phase in the mixing layer of the saturated zone. Major time dependent output from the TSOURC modules; used in the WATEX module. Calculated using equation (3.9.16) in SENES Vol. 3. A maximum value of

$$WCONC(2,3,3) = 5 \times 10^{-5} \times 10^{3} \times THORCF \text{ [Bq } m^{-3}\text{]}$$

is assigned. If THDISM > THSOL, WCONC(2,3,3)=0 using equation (3.9.19)

WCONC(2,4,3) AQ. TH IN BOTTOM SAT. ZONE [Bq m^{-3}]. The concentration of thorium in the aqueous phase in the bottom layer of the saturated zone. Major time dependent output from the TSOURC modules; used in the WATEX module. Calculated using equation (3.9.16) in SENES Vol. 3. A maximum value of

$$WCONC(2,4,3) = 5 \times 10^{-5} \times 10^{3} \times THORCF \text{ [Bq } m^{-3}\text{]}$$

is assigned.

WCONC(3,2,3) AQ. PB-210 BOTTOM UNSAT. ZONE [Bq m^{-3}]. The concentration of lead-210 in the aqueous phase at the bottom of the unsaturated zone. Intermediate time dependent variable calculated in the TSOURC modules. Calculated using equations (3.11.2) and (3.11.6) in SENES Vol. 3.
NOTE: See DDD 1.5.2.7 for the initial condition.

WCONC(3,3,3) AQ. PB-210 MIXING LAYER [Bq m^{-3}]. The concentration of lead-210 in the aqueous phase of the mixing layer of the saturated zone. Major time dependent output from the TSOURC modules; used in the WATEX module. Calculated using equation (3.11.13) in SENES Vol. 3.
NOTE: See DDD 1.5.3.5 for the intial condition.

WCONC(3,4,3) AQ. PB-210 BOTTOM SAT. ZONE [Bq m^{-3}]. The concentration of lead-210 in the aqueous phase in the bottom layer of the saturated zone. Major time dependent output from the TSOURC modules; used in the WATEX module. Calculated using equation (3.11.19) in SENES Vol. 3.
NOTE: See DDD 1.5.3.8 for the initial condition.

WCONC(3,j,2),(j=3,4) as WCONC(3,j,3) above, but for TIME=t-Δt rather than TIME=t

WCONC(4,2,3) AQ. RA BOTTOM UNSAT. ZONE [Bq m^{-3}]. The concentration of radium-226 in the aqueous phase at the bottom of the unsaturated zone. Intermediate time dependent variable calculated in the TSOURC modules. Calculated using equations (3.10.21) and (3.10.22) in SENES Vol. 3.
NOTE: See DDD 1.4.3.5 for the initial condition.

WCONC(4,3,3) AQ. RA IN MIXING LAYER [Bq m^{-3}]. The concentration of radium-226 in the aqueous phase in the mixing layer of the saturated zone. Major time dependent output from the TSOURC modules; used in the WATEX module. Calculated using equation (3.10.31) in SENES Vol. 3.
NOTE: See DDD 1.4.4.5 for the initial condition.

WCONC(4,4,3) AQ. RA IN BOTTOM SAT. ZONE [Bq m^{-3}]. The concentration of radium-226 in the aqueous phase at the bottom of the saturated zone. Major time dependent output from the TSOURC modules; used in the WATEX module. Calculated using equation (3.10.37) in SENES Vol. 3.
NOTE: See DDD 1.4.4.8 for the initial condition.

WCONC(4,j,2),(j=3,4) as WCONC(4,j,3) above, but for TIME=t-Δt rather than TIME=t

WCONC(6,2,3) CONC. OF S04 AQ. AT BOTTOM OF UNSAT. ZONE FROM PYRITE [mol m^{-3}]. Concentration of sulphate ions in the aqueous phase at the bottom of the unsaturated zone, due to pyrite oxidation and downward movement of water (including sulphate in precipitation), as a function of time. Intermediate variable calculated in the TSOURC modules. Calculated using equation (3.3.14) in SENES Vol. 3.

NOTE: A background value of 0.1 [mol m^{-3}] is included, except for the initial condition (inspection of the UTAP2 code).

NOTE: The background value is deliberately inconsistent with the 0.071 [mol m^{-3}] selected in WATEX.

NOTE: WCONC(6,2,3) has a minimum value of 1.0E-20 (inspection of the UTAP2 code).

WCONC(6,3,3) CONC. OF S04 AQ. IN MIXING LAYER FROM PYRITE [mol m^{-3}]. Concentration of sulphate ions in the aqueous phase in the mixing layer of the saturated zone, due to pyrite oxidation and downward movement of water (including sulphate in precipitation), as a function of time. Intermediate variable used in the TSOURC modules. Calculated using equation (3.4.5) in SENES Vol. 3.

WCONC(6,4,3) CONC. OF S04 AQ. IN BOTTOM LAYER FROM PYRITE [mol m^{-3}]. Concentration of sulphate ions in the aqueous phase in the bottom layer of the saturated zone, due to pyrite oxidation and downward movement of water (including sulphate in precipitation), as a function of time. Intermediate variable used in the TSOURC modules. Calculated using equation (3.5.2) in SENES Vol. 3.

WCONC(6,j,2),(j=3,4) as WCONC(6,j,3) above, but for TIME=t-Δt rather than TIME=t

WCONC(7,1,3) CONC. OF S04 AQ. AT GYPSUM-DEPLETED FRONT [mol m^{-3}]. Total concentration of sulphate ions in the aqueous phase at the bottom of the gypsum-depleted front of the unsaturated zone (from pyrite oxidation and downward movement of water as a function of time). Intermediate variable used in the TSOURC modules. Calculated using equations (3.3.15b) and (3.3.36) of SENES Vol 3. If the unsaturated layer is completely depleted of gypsum WCONC(7,1,3) = WCONC(7,2,3) = WCONC(6,2,3).

NOTE: The initial condition is WCONC(7,1,3)=0 (inspection of the UTAP2 code). See other comments in DDD 1.1.3.1.

WCONC(7,2,3) CONC. OF S04 AQ. BOTTOM UNSAT. ZONE [mol m^{-3}]. Total concentration of sulphate ions in the aqueous phase at the bottom of the unsaturated zone. Intermediate time dependent variable used in the TSOURC modules. Calculated using equation (3.3.40) of SENES Vol. 3 if no calcite is present and the unsaturated layer in not depleted of gypsum, from equation (3.3.60) if calcite is present and the unsaturated layer is not depleted of gypsum. If the unsaturated layer is completely depleted of gypsum WCONC(7,2,3)=WCONC(6,2,3).

NOTE: See DDDs 1.1.2.8 and 1.1.2.11 for additional comments that affect the calculation of WCONC(7,2,3).

WCONC(7,3,3) CONC. OF S04 AQ. IN MIXING LAYER [mol m^{-3}]. The total concentration of sulphate ions in the aqueous phase in the mixing layer of the saturated zone. Major time dependent output from the TSOURC modules; used in the LAKEPH module. Calculated using equation (3.4.7) of SENES Vol 3 if gypsum is not totally depleted from the mixing layer, and from equation (3.4.12) if the mixing layer is

depleted of gypsum.
NOTE: It appears from the SENES documentation that if
GYPMIX at TIME=t-Δt $<$ GYPI and
GYPMIX at TIME=t $\geq$ GYPI
then WCONC(7,3,3) must be recalculated after the calculation of GYPMIX

WCONC(7,4,3) CONC. OF SO4 AQ. IN BOTTOM LAYER [mol m^{-3}]. The total concentration of sulphate ions in the aqueous phase in the bottom layer of the saturated zone. Time dependent variable from the TSOURC module; used in the LAKEPH module. Calculated using equation (3.5.4) of SENES Vol 3.

WCONC(8,2,3) CONC. OF CA AQ. BOTTOM UNSAT. ZONE [mol m^{-3}]. Concentration of calcium ions in the aqueous phase at the bottom of the unsaturated zone in the absence of calcite. Intermediate time dependent variable used in the TSOURC modules. Calculated using equations (3.3.39) and (3.3.40) of SENES Vol. 3.

WCONC(8,3,2) as WCONC(8,3,3) below, but for TIME=t-Δt rather than TIME=t

WCONC(8,3,3) CONC. OF CA AQ. IN MIXING LAYER [mol m^{-3}]. Concentration of calcium ions in the aqueous phase in the mixing layer of the saturated zone. Major time dependent output from the TSOURC modules; used in the LAKEPH module. Calculated using equations (3.4.6) and (3.4.7) of SENES Vol. 3 if gypsum has not been totally depleted from the mixing zone, and from equation (3.4.11) if there is no gypsum in the mixing zone.

WCONC(8,4,3) CONC. OF CA AQ. IN BOTTOM LAYER [mol m^{-3}]. Concentration of calcium ions in the aqueous phase in the bottom layer of the saturated zone. Major time dependent output from the TSOURC modules; used in the LAKEPH module. Calculated using equations (3.5.3) and (3.5.4) of SENES Vol. 3.

WCONC(9,2,3) CONC. FE(III) BOTTOM UNSAT. ZONE [mol m^{-3}]. Concentration of iron (III) in the aqueous phase at the bottom of the unsaturated zone. Intermediate time dependent variable used in the TSOURC modules. Calculated using equation (3.3.44) of SENES Vol. 3.

WCONC(10,3,3) CONC. FE(II) IN MIXING LAYER [mol m^{-3}]. Concentration of iron (II) in the aqueous phase in the mixing layer of the saturated zone. Intermediate time dependent variable used in the TSOURC modules. Calculated using equation (3.4.16) of SENES Vol. 3.

WCONC(10,4,3) CONC. FE(II) IN BOTTOM LAYER [mol m^{-3}]. Concentration of iron (II) in the aqueous phase in the bottom layer of the saturated zone. Intermediate time dependent variable used in the TSOURC modules. Calculated using equation (3.5.5) of SENES Vol. 3.

WCONC(10,j,2),(j=3,4) as WCONC(10,j,3) above, but for TIME=t-Δt rather than TIME=t

WCONC(nuc,3,3) see WCONC(1,3,3), WCONC(2,3,3), WCONC(3,3,3), WCONC(4,3,3) for nuc = nat-U, tot-Th, Ra-226, Pb-210, respectively.

WCONC(nuc,4,3) see WCONC(1,4,3), WCONC(2,4,3), WCONC(3,4,3), WCONC(4,4,3) for nuc = nat-U, tot-Th, Ra-226, Pb-210, respectively.

WFLOC FRAC. OF WATER LOCAL [-]. Fraction of annual water consumption that is from local drinking water. Receptor specific input parameter used in the DOSE modules and sampled from:
Triangular (0.4, 0.6, 0.9) - critical receptor
Triangular (0.8,0.9,1.0) - average receptor

WIRC CARIBOU WATER INTAKE RATE [m^3 d^{-1}]. The average daily water intake rate for caribou. Input parameter used in the DOSE module and sampled from:
Triangular (7.7×10^{-3},11.5×10^{-3},15.3×10^{-3}).

WIRM	MOOSE WATER INTAKE RATE [$\mathrm{m}^3\ \mathrm{d}^{-1}$]. The average daily water intake rate for moose. Input parameter used in the DOSE module and sampled from: Triangular (0.024, 0.036, 0.048).
WKDPB	LAKE KD FOR PB [$\mathrm{m}^3\ \mathrm{g}^{-1}$]. Distribution coefficient from water to lake sediment for lead. Input parameter used in the WATEX module and sampled from: Log Normal (1.5×10^{-2}, 2.5, 1.0×10^{-3}, 0.23)
WKDRA	LAKE KD FOR RA [$\mathrm{m}^3\ \mathrm{g}^{-1}$]. Distribution coefficient from water to lake sediment for radium. Input parameter used in the WATEX module and sampled from: Log Normal (6.5×10^{-3}, 2.5, 0.4×10^{-3}, 0.10)
WKDTH(n)	LAKE KD FOR TH [$\mathrm{m}^3\ \mathrm{g}^{-1}$]. Distribution coefficient from water to lake sediment for thorium. Parameter used in the WATEX module and calculated from equation 10.13 of SENES Vol. 3 for each lake node n, n=1,8) if WATPH $\geq$ 4.0, and sampled from: Constant (2.0×10^{-3}) if WATPH < 4.0
WKDU	LAKE KD FOR U [$\mathrm{m}^3\ \mathrm{g}^{-1}$]. Distribution coefficient from water to lake sediment for uranium. Input parameter used in the WATEX module and sampled from: Log Normal (4.5×10^{-3}, 2.2, 0.4×10^{-3}, 4.8×10^{-2})
WMOC(nuc)	WATER - MOOSE CONC. [Bq g^{-1}(wet)]. Concentration of the radionuclide "nuc" in moose flesh due to the water pathway (nuc = U-nat, Th-tot, Ra-226, Pb-210). Time dependent parameter used in the DOSE module and calculated from equation (12.4) of SENES Vol. 3.
WSIGD(n)	RATE OF SEDIMENT BURIAL [$\mathrm{g}\ \mathrm{m}^{-2}\ \mathrm{a}^{-1}$] Rate of sediment burial or removal from the active exchange zone. Intermediate parameter used in the WATEX model and calculated from: WSIGD(n) = WSIGS(n) x BURYF , equation 10.12 of SENES Vol. 3. NOTE: See DDD 3.3.5 for a correction for WSIGD of the first lake.
WSIGS(n)	RATE OF SEDIMENTING MATERIAL REMOVAL [$\mathrm{g}\ \mathrm{m}^{-2}\ \mathrm{a}^{-1}$]. Rate of removal of sedimenting material from the water column of the lake between nodes (n-1) and n in the watershed. Input parameter used in WATEX and sampled from: Constant (0.0) n=1,3,5,6,8 (rivers) Triangular (95, 230, 615) n=2 (105, 260, 765) n=4 (85, 210, 515) n=7
WTMIXD	SEDIMENT ZONE THICKNESS [m]. Thickness of the sediment exchange zone in the lakes of the watershed. Input parameter used in WATEX and sampled from: Constant (0.05)
WTRHOS	SEDIMENT SOLID DENSITY [$\mathrm{g}\ \mathrm{m}^{-3}$]. Density of the stabilized sediment solids. Input parameter used in WATEX and sampled from: Constant (1.84×10^6)
WTSEG	NODE NUMBER [-]. Node number for the end of the nth segment in the watershed (10 maximum). Counter used in the WATEX module.
WTSFLX	RATIO OF RN FLUXES FROM FROZEN AND UNFROZEN TAILINGS [-] The ratio of the Rn-222 flux from frozen tailings to the flux from the same tailings when they are not frozen. Input parameter used in the RADON module and sampled from: Log Normal (0.02,2.0,0.002,0.2)
WTSO4B	BACKGROUND SULPHATE LEVEL [$\mathrm{mol}\ \mathrm{m}^{-3}$]. The natural background sulphate concentration level in freshwater flow. Input parameter used

in the LAKEPH module and sampled from:

Constant (0.071)

NOTE: The background value is deliberately inconsistent with the 0.1 [mol m^{-3}] selected in TSOURC (equation 3.3.14).

X(nuc,n) X PARAMETER USED IN WATEX [Bq]. Intermediate parameter used in the calculation of WATRW and WATRS in the WATEX module. This is a time dependent parameter defined in in an equation below equations (10.32) and (10.33)(nuc=nat-U, tot-Th) or (for nuc=Ra-226, Pb-210) by an equation near the bottom of page 10-29 using expressions given on page 10-30 in SENES Vol. 3.

NOTE: The expressions on page 10-30 of SENES Vol. 3 are incorrect. The corrected versions are supplied in a letter from SENES (1986-12-02).

X230LA ACTIV. FRACT. TH-230 IN SOLU. TH [-]. The fraction of Th-230 in soluble thorium on the basis of activity. Parameter calculated in the TSOURCE module and used in the WATEX module. The equation is not given in SENES Vol. 3, but the parameter was calculated using the definition:

X230LA = 1.0 - X232LA

X230LM MOLE FRACT. TH-230 [-]. Mole fraction of Th-230 in soluble thorium. Parameter calculated and used in the TSOURCE modules. Calculated from equation (3.7.27) of SENES Vol. 3.

X232LA ACTIV. FRACT. TH-232 IN SOLU. TH [-]. The fraction of Th-232 in soluble thorium on the basis of activity. Parameter calculated in the TSOURCE module and used in the DOSE module. Calculated using a combination of equations (3.7.26) and (3.7.29) of SENES Vol. 3.

X232LA = (T232SO x T232CF)/(T230SO x T230CF + T232SO x T232CF)

X232LM MOLE FRACT. TH-232 [-]. Mole fraction of Th-232 in soluble thorium. Parameter calculated and used in the TSOURCE modules. Calculated from equation (3.7.28) of SENES Vol. 3.

X232SA ACTIV. FRACT. TH-232 IN SURF. SOLID TH [-]. The fraction of Th-232 in solid thorium in the unsaturated zone (on the basis of activity). Time dependent parameter calculated in the TSOURC module and used in the DOSE module and calculated using equation (3.9.11) of SENES Vol. 3.

NOTE: See DDD 1.3.2.5C for the initial condition.

XBAR MOLE FRACT. RA-226 IN BASO4 SOLID [-]. The solid phase mole fraction of Ra-226 in $BaSO_4$ at TIME=t. Intermediate variable used in the TSOURC modules and calculated using equation (3.10.18) of SENES Vol. 3. At TIME=0, XBAR ≡ XRADI (pg. 3-84, SENES Vol. 3).

XLEAD MOLE FRACT. PB-210 [-]. Mole fraction of $^{210}PbSO_4$ in the lead sulphate, corrected for decay of Pb-210. Intermediate time dependent variable used in the TSOURC modules and calculated using an equation below equation (3.11.2) of SENES Vol. 3.

XLIME INIT. MASS FRACT. LIME [-]. Initial mass fraction of $CaCO_3$ in tailings. A scenario dependent constant used in the TSOURC modules and sampled from:

Constant (0.00) or
Constant (0.01)

The value of XLIME determines the scenario. If no limestone has been added XLIME = 0. If limestone has been added, the only case considered is when XLIME =0.01 (i.e., the limestone is 1% of the total tailings mass). Methods of calculation of a number of the TSOURC modules parameters are affected by the choice of senario. See SENES Vol. 3, section 2.7

XPBI	INIT. MOLE FRACT. PB-210 [-]. Initial mole fraction of $^{210}PbSO_4$ in the lead sulphate. Parameter used in the TSOURC modules and calculated from equations (3.7.48) and (3.7.50) of SENES Vol. 3.
XRAD	MOLE FRACT. RA-226 [-]. Mole fraction of $^{226}RaSO_4$ in the barium sulphate, corrected for decay of Ra-226. Intermediate time dependent variable used in the TSOURC modules and calculated using equation (3.10.19) of SENES Vol. 3.
XRADI	INIT. MOLE FRACT. RA-226 [-]. Initial mole fraction of $^{226}RaSO_4$ in the barium sulphate. Input parameter used in the TSOURC modules and sampled from: Triangular (2.5×10^{-6}, 3.5×10^{-6}, 4.5×10^{-6})
XRGWAT	DISCHARGE DISTANCE [m]. The distance between the tailings dam and the point where the subsurface flow is discharged to the watershed. Input parameter used in the GWATER module and sampled from: Triangular (25., 35., 200.)
XURANI	MOL. FRACT. U308 IN PYRITE [-]. The fraction (on a molar basis) of U_3O_8 in the initial pyrite component of the tailings. Intermediate parameter used in the TSOURC modules, and calculated using equation (3.7.7) of SENES Vol.3.
Y(nuc,n)	Y PARAMETER USED IN WATEX [Bq]. Intermediate parameter used in the calculation of WATRW and WATRS in the WATEX module. This is a time dependent parameter defined in in an equation below equations (10.32) and (10.33)(nuc=nat-U, tot-Th) or (for nuc=Ra-226, Pb-210) by an equation near the bottom of page 10-29 using expressions given on page 10-30 in SENES Vol. 3. NOTE: The expressions on page 10-30 of SENES Vol. 3 are incorrect. The corrected versions are supplied in a letter from SENES (1986-12-02).
YDEN(v)	YIELD DENSITY [g(wet weight) m^{-2}]. Mass of vegetation types v (v=1,2,3,4,5; above-ground and below-ground vegetables,summer forage, browse and lichen) produced per unit area of ground. Input parameter used in the VEGCON module, and sampled from: Uniform (1000, 3000) (v=1,2) Uniform (500, 1000) (v=3,4) Uniform (400, 600) (v=5)
ZAVG(nuc)	AVG. ACTIVITY IN SOIL LAYER [Bq]. The average value of ZTOT for the time interval between t and t-Δt. Intermediate time dependent variable used in the SOIL module. NOTE: See DDD 2.4.4 for additional comments.
ZMDT(nuc)	INITIAL RADIONUCLIDE ACTIVITIES IN THE SOIL LAYERS [Bq]. The activity of the nuclide (nuc) (nuc= Ra-226, Pb-210, tot-Th, nat-U) in each soil layer (assumed independent of the soil layer) at time t = -Δt. Input parameters used in the SOIL module and sampled from: Constant (0.0) Note: These values are not given in SENES Vol. 3, and but were confirmed by SENES in a letter (1986-10-15).
ZTOT(nuc,sla,loc)	RADIONUCLIDE ACTIVITY SOIL LAYER [Bq]. The activity of the radionuclide (nuc) (nuc= Ra-226, Pb-210, tot-Th, nat-U) in the soil layer (sla), (sla=1,NLAYER) at receptor site "loc" at time t. This is an intermediate time-dependent variable used in the SOIL module and calculated from a finite-difference equation (equation (6.8)) of SENES Vol. 3. NOTE: See also DDDs 2.4.3 and 2.4.5 for modifications to the equations used to calculate ZTOT.

APPENDIX D. SUMMARY OF THE WALKTHROUGHS FOR THE SPECIFICATIONS

A walkthrough is defined by Page-Jones[1] to be "a peer group review of a product for the purpose of finding any deficiencies in that product". The object of a walkthrough is to find problems or potential problems, and not to find solutions. The attendees are challenged to find flaws.

Three of the attendees have special roles. The presenter presents the product being reviewed and describes its function and how it works. The coördinator keeps the meeting focussed on the purpose of the walkthroughs. Finally the recorder writes down each question and critical comment that arise during the meeting. All participants contribute to the walkthrough of the product, identifying missing elements, unworkable segments, special cases that may not be treated properly, inconsistent logic, and so forth.

The specifications from the uranium tailings model were subjected to a series of formal walkthroughs. The participants were provided with the relevant information required to assess the specifications, including the appropriate sections from the SENES report[2], a copy of the data dictionary, and the existing (preliminary) specifications.

At the end of the meeting, the participants were asked to either accept or reject the product. If a product was rejected, follow-up walkthroughs were held until the product was judged to be acceptable. A product can be accepted if, and only if, all participants concur. Often some parts of the product were accepted, while other parts were rejected (and required a follow-up).

Most walkthroughs involved four participants, usually chosen on the basis of their experience with a specific component model and/or their experience with system analysis and programming. For expediency, some of the later walkthroughs involved fewer participants.

A summary of the walkthroughs is presented in Table D-1, and is organized by the groups in which the specifications were examined. Most walkthroughs dealt with about 5 to 15 data flow diagrams and/ or data dependency diagrams, depending somewhat on the complexity of the product and the natural groupings of the figures. A total of 251 specifications were approved in 36 walkthroughs[3]. Most walkthroughs lasted about one

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1/ Page-Jones, M., 1980. The Practical Guide to Structured Systems Design; YOURDON Inc., New York, P. 294.

2/ SENES, 1986. Probabilistic Model Development for the Assessment of the Long-Term Effects of Uranium Mill Tailings in Canada - Phase III; Volume 3 - Tailings Assessment Program (UTAP) Component Model Documentation. Contract report prepared under contract #0SQ85-00182 for the National Uranium Tailings Program, Canada Centre for Mineral and Energy Technology, Energy, Mines and Resources Canada, 555 Booth Street, Ottawa, Ontario, K1A 0G1.

3/ DDD 2.3.7A, added late in the first comparison, was not included in these walkthroughs.

hour, although the lead preparation time could take several hours per participant.

In an ideal environment, the specification walkthrough process should begin once a complete set of specifications are available, and proceed downwards from the uppermost overview data flow diagram. It is also desirable to use the same participants, and to hold the meetings over a short time frame, to ensure continuity of the process. Unfortunately an ideal environment seldom exists. For the walkthroughs of the uranium tailings model, time constraints required that walkthroughs be started before all specifications were complete, and different components of the model were examined as they became available. Delays in the resolution of some questions, required to complete some specifications, also contributed to the protracted time frame and a changeover in participants. Two steps were taken to offset these difficulties:

(1) One or two of the participants (TA and BG) were involved in all walkthroughs.
(2) A final review was held, covering all figures in the specifications (including any that had been previously accepted).

Although the walkthroughs of the specifications were time-consuming, we feel that they provided positive benefits to this project. Many errors and ambiguities in the specifications were trapped before they could affect the design and programming phases of the project. In some instances, problems in the original documentation were also exposed. The specifications for the uranium tailings model provide an important bridge between the scientific description of the model and the resultant code, and walkthroughs serve as a "peer review" of the specifications. We strongly recommend the continued use of formal walkthroughs (and the preparation of specifications) for other projects of this nature.

TABLE D1

Summary of Walkthroughs for the Uranium Tailings Specifications

Code*	Date	Description and comments	Reviewers**	Number of Figures	
				Accepted	Rejected
1-1	86-09-12	Dust and Rn gas emission Fig. 2.1, 2.2, 2.2.1-2.2.4	TA, KF, BG, RL	6	0
1-1R	87-01-20	As in 1-1; final review	BG, RJ	-	-
2-1	86-09-12	Watershed concentrations Fig. 4.1, 4.1.1-4.1.12	TA, BG, RL, GS	13	0
2-1R	87-01-30	As in 2-1; final review. Figures renumbered to 3.3, 3.3.1-3.3.9 inclusive and 8 new figures added.	BG, RL	8	0
3-1	86-10-22	Vegetation concentrations Fig. 2.6	TA, KF, BG, RL	0	1
3-1R	87-01-20	As in 3-1; final review	BG, RL	1	0
4-1	86-10-22	Groundshine dose Fig. 2.5, 2.5.1-2.5.4	TA, BG, RL, DM	0	5
4-1R	87-02-06	As in 3-1; final review. Three figures were added, (2.5.5-2.5.7).	BG, RL	8	0
5-1	86-10-23	Soil concentrations Fig. 2.4, 2.4.1-2.4.5	TA,BG,RL	0	6
5-1R	87-01-20	As in 5-1; final review. One figure was added (2.4.6).	BG, RL	7	0
6-1	86-10-23	Atmospheric transport Fig. 2.3	TA, BG, RL, AS	0	1
6-1R	87-01-20	As in 6-1; final review. Seven figures were added (2.3.1-2.3.7)	BG, RL	8	0
7-1	86-10-24	Groundwater transport Fig. 3.1, 3.1.1-3.1.7	TA, BG, RL, TM	4	4
7-1R	87-01-20	As in 7-1; final review	BG, RL	4	0
8-1	86-10-24	Lake pH Fig. 4.3, 4.3.1-4.3.7	TA, BG, RL, AS	5	3
8-1R	87-01-26	As in 8-1; final review. Figures renumbered to 3.2, 3.2.1-3.2.7. One figure added (3.2.5A)		4	0
9-1	86-11-07	Source-time independent variables; Fig. 1.1.1, 1.1.1.1-1.1.1.4, 1.1.2.1-1.1.2.2	TA, BG, RL, DM	7	0
9-2	86-11-13	Source-chemical composition Fig. 1.1.2, 1.1.2.3-1.1.2.13	TA, DM, PV	10	2

Code*	Date	Description and comments	Reviewers**	Number of Figures	
				Accepted	Rejected
9-3	86-11-19	Source-pH in layers 1 and 3 Fig. 1.1.3, 1.1.3.1-1.1.3.2, 1.1.4, 1.1.4.1-1.1.4.7	TA, BG, DM, PV	7	4
9-4	86-11-21	Source-pH in layer 4 and uranium concentrations Fig. 1.1, 1.2, 1.2.1-1.2.6, 1.1.5, 1.1.5.1-1.1.5.5	TA, BG, DM, PV	14	0
9-1R	86-12-15	As in 9-1 to 9-4; first repeat review. Fig. 1.1.2 was rejected.	TA, BG, DM, PV	5	1
9-2R	87-01-12	As in 9-1 to 9-4 (with emphasis on Fig. 1.1.2); final review	TA, RL	1	0
10-1	86-11-26	Source-constant thorium parameters Fig. 1.3.1, 1.3.1.1-1.3.1.12	TA, BG, PV	13	0
10-2	86-11-27	Source-thorium concentrations Fig. 1.3, 1.3.2, 1.3.2.1-1.3.2.8	TA, BG, DM	7	3
10-1R	87-01-09	As in 10-1 and 10-2; final review. Five figures were added (1.3.1.7A and B; 1.3.2.1A and B; 1.3.2.5A, B and C; 1.3.2.6A and B)	BG, RL	8	0
11-1	86-11-28	Source-radium in layer 1 and barium. Fig. 1.4.1, 1.4.1.1-1.4.1.4, 1.4.2, 1.4.2.1-1.4.2.6	TA, DM, PV	12	0
11-2	86-12-04	Source-radium conc. in layer 3 Fig. 1.4.3, 1.4.3.1-1.4.3.5	TA, BG, DM	6	0
11-3	86-12-09	Source-radium in sat. zone Fig. 1.4, 1.4.4, 1.4.4.1-1.4.4.8	TA, BG, PV	7	3
11-1R	87-01-09	As in 11-1 to 11-3; final review. One figure added (1.4.4.4B)	BG, RL	4	0
12-1	86-12-05	Source-lead conc. in unsat. zone. Fig. 1.5.1, 1.5.1.1-1.5.1.3, 1.5.2, 1.5.2.1-1.5.2.7	TA, BG, DM	12	0
12-2	86-12-09	Source-lead conc. in sat. zone Fig.1.5, 1.5.3, 1.5.3.1-1.5.3.8	TA, DM, PV	8	2
12-1R	87-01-09	As in 12-1 and 12-2; final review. One figure added (1.5.3.4B)	BG, RL	3	0
13-1	87-01-16	Erosion model; final review Fig. 1.6, 1.6.1, 1.6.1.1-1.6.1.11, 1.6.2, 1.6.2.1-1.6.2.7, 1.6.3, 1.6.3.1-1.6.3.10	BG, RL	32	0

Code[*]	Date	Description and comments	Reviewers[**]	Number of Figures	
				Accepted	Rejected
14-1	87-01-09	Internal dose models Fig. 5.0, 5.1, 5.1.1, 5.1.2, 5.1.2.1-5.1.2.5, 5.1.3, 5.1.3.1-5.1.3.3, 5.1.4, 5.1.5, 5.1.5.1-5.1.5.3, 5.2, 5.2.1-5.2.2, 5.3, 5.4	BG, RL	0	23
14-1R	87-01-09	As in 14-1; final review. All figures renumbered to 4.0, 4.1, etc.	BG, RL	23	0
15-1	87-02-02	Overview and high-level figures. Fig. 0, 1.0, 2.0, 3.0, 4.0 (repeated).	BG, RL	4	0
			TOTAL	251	58

[*] The first number of the code identifies a set of related specification figures; for example the series starting with 10 refer to source term specifications involving thorium. The second number refers to either a subset or a repeat walkthrough; for example 10-1 is the first of two subsets, and 10-1R is the first repeat walkthrough.

[**] Reviewers were T.H. Andres (TA), K. Frech (KF), B.W. Goodwin (BG), R.J. Lemire (RL), D.B. McConnell (DM), T.W. Melnyk (TM), G.R. Sherman (GS), A.M.M. Skeet (AS) and P. Vilks (PV)